



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 12:50 pm BST

PDB ID : 8Q7Z / pdb_00008q7z
EMDB ID : EMD-18168
Title : Structure of the G. gallus 80S non-rotated ribosome
Authors : Nurullina, L.; Jenner, L.; Yusupov, M.
Deposited on : 2023-08-17
Resolution : 2.50 Å(reported)
Based on initial model : 7O7Z

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

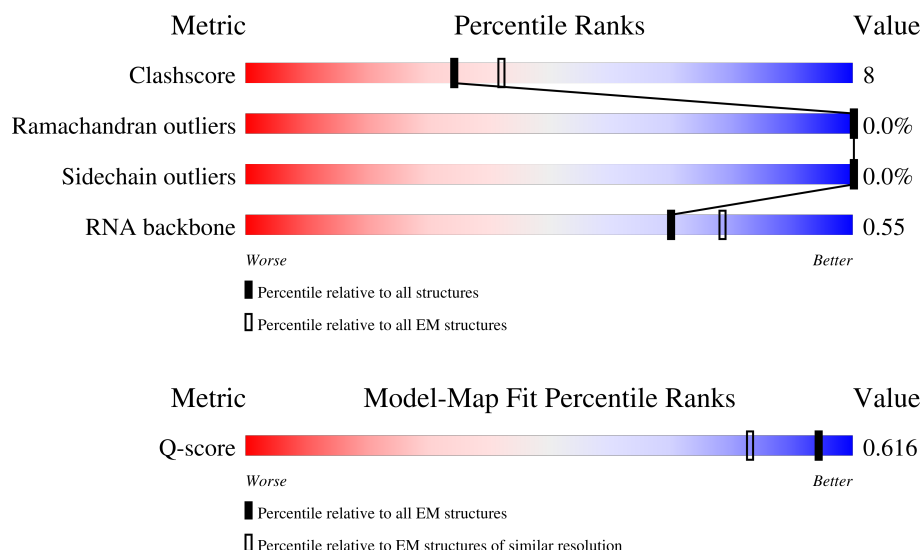
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B5	4441	
2	B8	157	
3	B7	119	

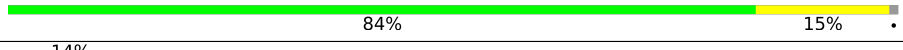
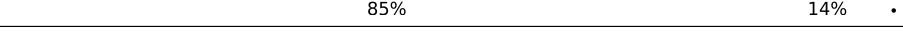
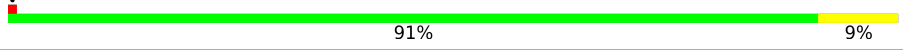
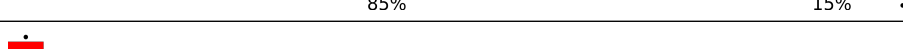
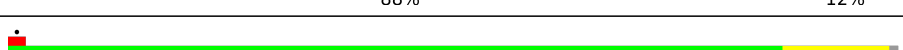
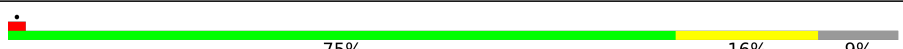
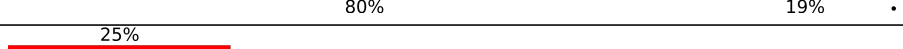
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Mol	Chain	Length	Quality of chain
4	Az	25	
5	BA	257	
6	BB	403	
7	BC	421	
8	BD	297	
9	BE	298	
10	BF	246	
11	BG	266	
12	BH	192	
13	BI	214	
14	BJ	178	
15	BL	211	
16	BM	131	
17	BN	204	
18	BO	203	
19	BP	184	
20	BQ	187	
21	BR	196	
22	BS	176	
23	BT	160	
24	BU	128	
25	BV	140	
26	BW	157	
27	BX	155	
28	BY	145	

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Mol	Chain	Length	Quality of chain
29	BZ	136	
30	Ba	148	
31	Bb	71	
32	Bc	115	
33	Bd	176	
34	Be	135	
35	Bf	110	
36	Bg	117	
37	Bh	123	
38	Bi	105	
39	Bj	97	
40	Bk	70	
41	Bl	51	
42	Bm	128	
43	Bo	105	
44	Bp	92	
45	Br	138	
46	A2	1823	
47	Aa	264	
48	AA	84	
49	AB	69	
50	Ab	264	
51	Ad	263	
52	AD	133	
53	AE	115	

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Mol	Chain	Length	Quality of chain
54	Af	249	
55	Ag	194	
56	Ah	207	
57	Ai	194	
58	Ak	158	
59	Am	151	
60	An	151	
61	At	119	
62	Au	84	
63	Av	130	
64	Aw	143	
65	Ax	131	
66	AZ	296	
67	Ap	146	
68	AC	156	
69	Ae	204	
70	AF	317	
71	AG	171	
72	Aj	165	
73	Al	132	
74	Ao	145	
75	Ar	152	
76	As	145	
77	Ay	125	
78	Ac	243	

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Mol	Chain	Length	Quality of chain
79	V	76	72% 34% 53% 13%
80	Aq	135	36% 64% 36%

2 Entry composition [i](#)

There are 83 unique types of molecules in this entry. The entry contains 216968 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B5	3562	Total	C	N	O	P	0	0
			76444	34065	13971	24846	3562		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3295	UY1	U	modified residue	GB KT445934.2

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B8	157	Total	C	N	O	P	0	0
			3338	1490	588	1103	157		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B7	119	Total	C	N	O	P	0	0
			2536	1130	449	838	119		

- Molecule 4 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Az	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	BA	248	Total	C	N	O	S	0	0
			1898	1191	387	314	6		

- Molecule 6 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	398	Total	C	N	O	S	0	0
			3209	2042	603	550	14		

- Molecule 7 is a protein called 60S ribosomal protein L4 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	361	Total	C	N	O	S	0	0
			2888	1816	574	484	14		

- Molecule 8 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	BD	296	Total	C	N	O	S	0	0
			2388	1506	437	433	12		

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BE	224	Total	C	N	O	S	0	0
			1811	1161	353	295	2		

- Molecule 10 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	BF	234	Total	C	N	O	S	0	0
			1939	1245	377	309	8		

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BG	210	Total	C	N	O	S	0	0
			1704	1089	326	284	5		

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BH	192	Total	C	N	O	S	0	0
			1533	962	288	277	6		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BI	205	Total	C	N	O	S	0	0
			1654	1050	322	268	14		

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BJ	170	Total	C	N	O	S	0	0
			1362	861	255	241	5		

- Molecule 15 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BL	210	Total	C	N	O	S	0	0
			1710	1072	354	279	5		

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BM	130	Total	C	N	O	S	0	0
			1077	688	209	172	8		

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BN	203	Total	C	N	O	S	0	0
			1700	1071	359	266	4		

- Molecule 18 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BO	201	Total	C	N	O	S	0	0
			1643	1058	321	259	5		

- Molecule 19 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BP	155	Total	C	N	O	S	0	0
			1259	788	244	218	9		

- Molecule 20 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BQ	187	Total	C	N	O	S	0	0
			1503	939	314	245	5		

- Molecule 21 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BR	180	Total	C	N	O	S	0	0
			1503	930	325	238	10		

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BS	176	Total	C	N	O	S	0	0
			1464	931	286	236	11		

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BT	159	Total	C	N	O	S	0	0
			1299	825	252	216	6		

- Molecule 24 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BU	100	Total	C	N	O	S	0	0
			817	523	143	149	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BV	134	Total	C	N	O	S	0	0
			993	625	187	176	5		

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BW	67	Total	C	N	O	S	0	0
			560	356	107	94	3		

- Molecule 27 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 28 is a protein called Ribosomal protein L26 like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BY	133	Total	C	N	O	S	0	0
			1106	694	224	185	3		

- Molecule 29 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ba	147	Total	C	N	O	S	0	0
			1179	748	240	187	4		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bb	70	Total	C	N	O	S	0	0
			582	360	126	94	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bc	95	Total	C	N	O	S	0	0
			738	468	131	133	6		

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Bd	105	Total	C	N	O	S	0	0
			867	549	168	148	2		

- Molecule 34 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Be	130	Total	C	N	O	S	0	0
			1074	681	219	169	5		

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Bf	110	Total	C	N	O	S	0	0
			886	559	178	144	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bf	103	VAL	-	insertion	UNP A0A8V0YS49

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Bg	108	Total	C	N	O	S	0	0
			860	540	178	137	5		

- Molecule 37 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 38 is a protein called Large ribosomal subunit protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bi	100	Total	C	N	O	S	0	0
			821	515	173	127	6		

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bj	86	Total	C	N	O	S	0	0
			704	432	155	112	5		

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 41 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	50	Total	C	N	O	S	0	0
			442	281	96	64	1		

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Bm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 43 is a protein called Ribosomal protein L36a like.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Bo	105	Total	C	N	O	S	0	0
			861	540	177	138	6		

- Molecule 44 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Bp	91	Total	C	N	O	S	0	0
			706	445	134	120	7		

- Molecule 45 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Br	126	Total	C	N	O	S	0	0
			1025	635	218	169	3		

- Molecule 46 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A2	1676	Total	C	N	O	P	0	0
			35806	16005	6419	11706	1676		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1206	B8N	U	modified residue	GB KT445934.2
A2	1295	4AC	C	modified residue	GB KT445934.2
A2	1796	4AC	C	modified residue	GB KT445934.2

- Molecule 47 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Aa	213	Total	C	N	O	S	0	0
			1730	1098	309	309	14		

- Molecule 48 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	AA	83	Total	C	N	O	S	0	0
			657	410	125	115	7		

- Molecule 49 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AB	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 50 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Ab	219	Total	C	N	O	S	0	0
			1698	1099	291	299	9		

- Molecule 51 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Ad	262	Total	C	N	O	S	0	0
			2076	1324	387	357	8		

- Molecule 52 is a protein called Ribosomal protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	AD	57	Total	C	N	O	S	0	0
			452	279	99	73	1		

- Molecule 53 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AE	99	Total	C	N	O	S	0	0
			793	492	165	131	5		

- Molecule 54 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Af	227	Total	C	N	O	S	0	0
			1838	1144	367	320	7		

- Molecule 55 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Ag	187	Total	C	N	O	S	0	0
			1500	956	276	267	1		

- Molecule 56 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Ah	206	Total	C	N	O	S	0	0
			1685	1059	332	289	5		

- Molecule 57 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Ai	179	Total	C	N	O	S	0	0
			1495	953	299	241	2		

- Molecule 58 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ak	152	Total	C	N	O	S	0	0
			1236	784	233	213	6		

- Molecule 59 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 60 is a protein called Ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
An	138	IAS	ASP	modified residue	UNP Q5ZHW8

- Molecule 61 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	At	102	Total	C	N	O	S	0	0
			811	508	154	145	4		

- Molecule 62 is a protein called Small ribosomal subunit protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Au	84	Total	C	N	O	S	0	0
			640	394	118	124	4		

- Molecule 63 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Av	129	Total	C	N	O	S	0	0
			1035	659	193	177	6		

- Molecule 64 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Aw	142	Total	C	N	O	S	0	0
			1104	696	220	185	3		

- Molecule 65 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 66 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AZ	207	Total	C	N	O	S	0	0
			1626	1036	287	295	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AZ	2	ACE	-	acetylation	UNP P50890

- Molecule 67 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ap	141	Total	C	N	O	S	0	0
			1123	715	212	193	3		

- Molecule 68 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AC	74	Total	C	N	O	S	0	0
			611	386	117	101	7		

- Molecule 69 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 70 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	AF	311	Total	C	N	O	S	0	0
			2420	1526	422	460	12		

- Molecule 71 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	AG	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 72 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	96	Total	C	N	O	S	0	0
			812	532	143	131	6		

- Molecule 73 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Al	118	Total	C	N	O	S	0	0
			916	574	162	172	8		

- Molecule 74 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Ao	127	Total	C	N	O	S	0	0
			1044	663	197	177	7		

- Molecule 75 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ar	144	Total	C	N	O	S	0	0
			1191	748	241	201	1		

- Molecule 76 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	As	143	Total	C	N	O	S	0	0
			1115	698	216	199	2		

- Molecule 77 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ay	70	Total	C	N	O	S	0	0
			555	357	101	96	1		

- Molecule 78 is a protein called DNA-(apurinic or apyrimidinic site) lyase.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ac	225	Total	C	N	O	S	0	0
			1752	1117	315	313	7		

- Molecule 79 is a RNA chain called Phe tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	V	76	Total	C	N	O	P	0	0
			1628	727	302	524	75		

- Molecule 80 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Aq	134	Total	C	N	O	S	0	0
			1081	678	201	197	5		

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	B5	346	Total	Mg	0
			346	346	
81	B8	9	Total	Mg	0
			9	9	
81	B7	11	Total	Mg	0
			11	11	
81	BA	3	Total	Mg	0
			3	3	
81	BH	1	Total	Mg	0
			1	1	
81	BI	2	Total	Mg	0
			2	2	
81	BN	2	Total	Mg	0
			2	2	
81	BP	2	Total	Mg	0
			2	2	
81	BV	1	Total	Mg	0
			1	1	
81	Ba	1	Total	Mg	0
			1	1	
81	Bb	2	Total	Mg	0
			2	2	
81	Be	1	Total	Mg	0
			1	1	
81	Bf	1	Total	Mg	0
			1	1	
81	Bg	1	Total	Mg	0
			1	1	
81	Bj	1	Total	Mg	0
			1	1	
81	Bo	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
81	A2	104	Total 104	Mg 104	0
81	Ak	1	Total 1	Mg 1	0
81	An	3	Total 3	Mg 3	0
81	As	1	Total 1	Mg 1	0

- Molecule 82 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
82	Bg	1	Total 1	Zn 1	0
82	Bj	1	Total 1	Zn 1	0
82	Bm	1	Total 1	Zn 1	0
82	Bo	1	Total 1	Zn 1	0
82	Bp	1	Total 1	Zn 1	0
82	AE	1	Total 1	Zn 1	0
82	AG	1	Total 1	Zn 1	0

- Molecule 83 is water.

Mol	Chain	Residues	Atoms		AltConf
83	B5	4198	Total 4198	O 4198	0
83	B8	72	Total 72	O 72	0
83	B7	30	Total 30	O 30	0
83	Az	5	Total 5	O 5	0
83	BA	28	Total 28	O 28	0
83	BB	49	Total 49	O 49	0

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Mol	Chain	Residues	Atoms		AltConf
83	BC	45	Total 45	O 45	0
83	BD	22	Total 22	O 22	0
83	BE	11	Total 11	O 11	0
83	BF	24	Total 24	O 24	0
83	BG	15	Total 15	O 15	0
83	BH	15	Total 15	O 15	0
83	BI	13	Total 13	O 13	0
83	BJ	3	Total 3	O 3	0
83	BL	29	Total 29	O 29	0
83	BM	6	Total 6	O 6	0
83	BN	29	Total 29	O 29	0
83	BO	19	Total 19	O 19	0
83	BP	23	Total 23	O 23	0
83	BQ	24	Total 24	O 24	0
83	BR	9	Total 9	O 9	0
83	BS	21	Total 21	O 21	0
83	BT	21	Total 21	O 21	0
83	BU	2	Total 2	O 2	0
83	BV	17	Total 17	O 17	0
83	BW	4	Total 4	O 4	0
83	BX	5	Total 5	O 5	0

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Mol	Chain	Residues	Atoms		AltConf
83	BY	11	Total 11	O 11	0
83	BZ	5	Total 5	O 5	0
83	Ba	23	Total 23	O 23	0
83	Bb	11	Total 11	O 11	0
83	Bc	5	Total 5	O 5	0
83	Bd	9	Total 9	O 9	0
83	Be	17	Total 17	O 17	0
83	Bf	25	Total 25	O 25	0
83	Bg	9	Total 9	O 9	0
83	Bh	3	Total 3	O 3	0
83	Bi	8	Total 8	O 8	0
83	Bj	16	Total 16	O 16	0
83	Bl	5	Total 5	O 5	0
83	Bm	5	Total 5	O 5	0
83	Bo	15	Total 15	O 15	0
83	Bp	12	Total 12	O 12	0
83	Br	16	Total 16	O 16	0
83	A2	832	Total 832	O 832	0
83	Aa	10	Total 10	O 10	0
83	AA	8	Total 8	O 8	0
83	AB	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms		AltConf
83	Ab	11	Total 11	O 11	0
83	Ad	10	Total 10	O 10	0
83	AD	2	Total 2	O 2	0
83	AE	9	Total 9	O 9	0
83	Af	1	Total 1	O 1	0
83	Ah	7	Total 7	O 7	0
83	Ai	7	Total 7	O 7	0
83	Ak	10	Total 10	O 10	0
83	Am	4	Total 4	O 4	0
83	An	7	Total 7	O 7	0
83	At	3	Total 3	O 3	0
83	Au	2	Total 2	O 2	0
83	Av	10	Total 10	O 10	0
83	Aw	8	Total 8	O 8	0
83	Ax	4	Total 4	O 4	0
83	AZ	3	Total 3	O 3	0
83	Ap	1	Total 1	O 1	0
83	Ae	2	Total 2	O 2	0
83	AG	2	Total 2	O 2	0
83	Ar	1	Total 1	O 1	0
83	Ay	4	Total 4	O 4	0

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Mol	Chain	Residues	Atoms		AltConf
83	V	9	Total	O	0
			9	9	
83	Aq	4	Total	O	0
			4	4	

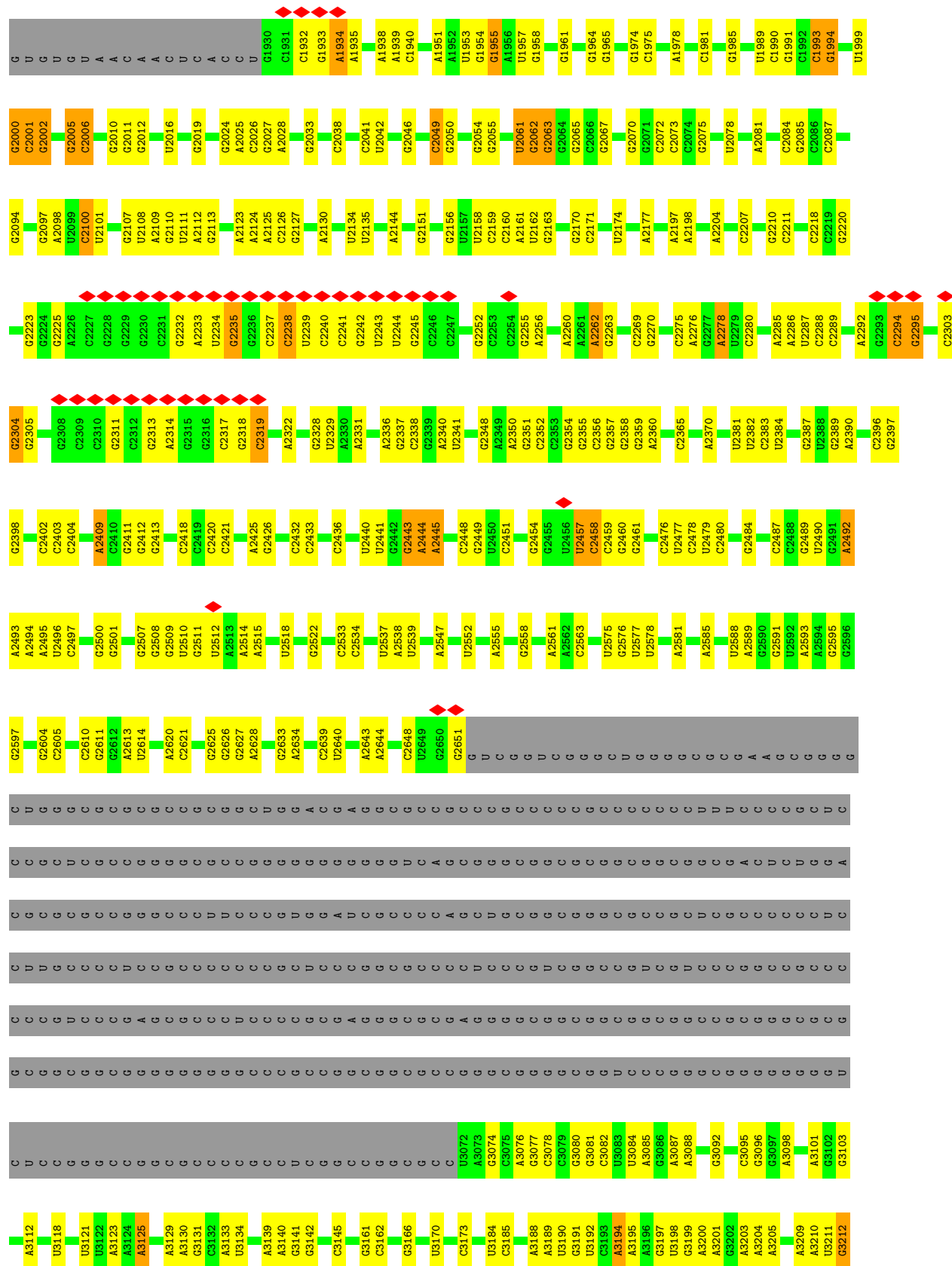
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

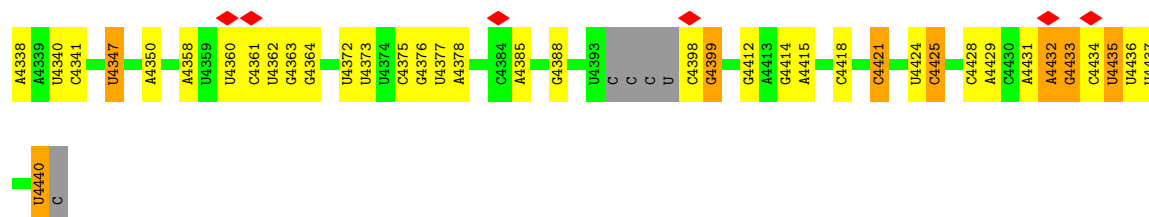
• Molecule 1: 28S rRNA



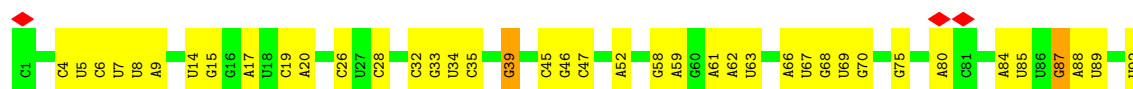




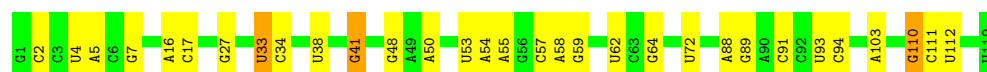
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A4265	C4183	G4080	A3991	G3916	C3792	G3710	G3618	C3550	C	A3420	A3214
C4266	A4184	U4081	G3992	A3915	U3793	A3711	U3619	C3551		G3421	G3230
C4267	C4185	G4082	G3993	A3916		A3712	A3620	G3552		G3422	
G4268	C4186	U4083	C4003	A3917	U3797	A3713	A3621	G3553		G3423	A3237
G4269	C4187	G4084	U4006	G3918	G3816	A3714	A3622	G3554		G3424	C3238
A4270	C4188	G4085	U4007	C3919	A3819	A3715	G3626	G3555		G3425	U3239
G4271	A4192	G4086	A4007	A3920	G3820	A3716	G3627	G3556		A3426	U3240
C4272	C4193	G4087	U4008	G3921	A3821	A3717	U3631	G3557		U3427	U3241
G4273	G4194	A4091	U4009	U3924	G3822	G3718	U3632	G3558		G3428	U3242
C4274	C4197	U4092	G4010	U3925	A3823	G3719	U3633	G3559		A3429	A3243
G4275		G4093	U4018	C3929	A3824	G3720	U3634	G3560		G3430	C3244
A4276	U4200	G4101	G4021	A3930	G3825	A3721	A3635	G3561		A3431	U3245
C4277	C4201	U4128	U4022	U3935	A3826	G3722	A3636	G3562		G3432	C3246
A4278	G4202	G4129	U4023	U3936	G3827	A3723	A3646	G3563		U3433	U3247
C4279	C4203	A4130	U4024	U3937	A3828	U3724	U3651	G3564		U3434	C3248
A4280	G4204	G4131	C4027	G3942	G3829	G3725	G3652	G3565		U3435	U3249
U4281	A4205	U4132	U4028	U3943	A3830	G3726	A3657	G3566		A3436	A3251
U4282	U4206	A4124	A4032	C3947	G3831	U3727	U3658	G3567		A3437	G3252
G4283	G4207	U4125	A4033	C3948	U3832	U3728	A3662	G3568		G3438	G3253
U4284	G4208	G4126	U4034	C3949	G3833	U3729	A3663	G3569		A3439	G3254
G4285	C4211	A4137	C4036	G3950	A3834	G3730	A3664	G3570		U3440	G3257
A4286	G4212	G4138	U4037	C3951	G3835	U3731	U3668	G3571		A3441	
C4287	A4207	U4139	U4038	U3952	G3836	G3732	G3671	A3575		A3442	U3275
G4288	G4208	A4140	A4039	A3953	A3837	U3733	U3672	C3580		A3443	
C4289	C4215	U4141	U4040	U3954	G3838	U3734	A3676	C3581		G3444	G3288
G4290	G4216	G4142	U4041	U3955	U3839	U3735	A3677	C3582		U3445	A3383
A4291	C4217	A4143	A4042	U3956	G3840	U3736	G3678	G3583		G3446	U3291
C4292	G4218	G4144	U4043	U3957	G3841	U3737	G3679	G3584		G3447	A3294
U4293	C4219	U4145	U4044	G3958	U3842	U3738	G3680	G3585		G3448	U13295
A4294	G4220	A4146	A4045	C3959	U3843	U3739	G3681	G3586		A3449	G3296
C4295	C4221	G4147	U4050	C3960	G3844	U3740	A3682	G3587		G3450	
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C4297	C4223	U4149	U4052	U3962	U3846	U3742	U3684	G3589		C3452	G3300
G4300	G4224	G4150	A4053	C3963	G3847	U3743	G3685	G3590		A3301	A3315
C4303	U4225	A4151	U4054	U3964	U3848	U3744	A3686	G3591		G3316	G3317
G4304	C4226	U4152	A4055	C3965	U3849	U3745	G3687	G3592		U3321	U3322
C4305	G4227	G4153	U4060	U3966	G3850	U3746	U3688	G3593		G3405	A3323
U4306	C4228	A4154	U4061	U3967	U3851	U3747	A3689	G3594		A3406	U3407
G4307	G4229	U4155	U4062	U3968	U3852	U3748	G3690	G3595		U3408	U3409
U4308	C4230	G4156	U4063	C3969	U3853	U3749	A3691	G3596		G3411	C3332
C4312	G4231	A4157	A4064	U3970	U3854	G3750	G3692	G3597		C3412	A3333
A4313	C4232	U4158	U4065	U3971	U3855	U3751	G3693	G3598		G	G3336
U4315	G4233	G4159	A4066	U3972	U3856	U3752	A3694	G3599		C	A3337
C4318	C4234	A4160	U4067	U3973	G3857	U3753	G3695	G3600		G	A3339
G4319	U4235	U4161	U4068	U3974	U3858	U3754	A3696	G3601		G	
C4320	C4236	G4162	A4069	C3975	U3859	U3755	G3697	G3602		U	
U4321	G4237	A4163	U4070	U3976	G3860	U3756	U3698	G3603		C	
C4323	C4238	U4164	U4071	U3977	U3861	U3757	A3699	G3604		G	
G4325	G4239	G4165	U4072	C3978	U3862	U3758	G3700	G3605		C	
A4326	C4240	A4166	A4073	U3979	U3863	U3759	C3701	G3606		C	
G4334	U4241	U4167	U4074	U3980	U3864	U3760	C3702	G3607		C	
C4335	C4242	G4168	U4075	C3901	U3865	U3761	G3703	C3608		C	
U4336	G4243	A4169	U4076	U3902	U3866	U3762	G3704	G3609		C	
A4337	C4244	U4170	U4077	U3903	U3867	U3763	G3705	G3610		C	
	G4245	G4180	U4078	C3904	U3868	U3764	U3706	G3611		C	
	C4253	C4181			U3869	U3765	U3707	G3612		C	
	C4254				U3870	U3766	U3708	A3613		C	
	C4255				U3871	U3767		G3614		C	
	C4256				U3872	U3768		A3615		C	
					U3873	U3769		G3616		C	
					U3874			G3617		C	
					U3875			A3618		C	
					U3876			G3619		C	
					U3877			A3620		C	
					U3878			G3621		C	
					U3879			A3622		C	
					U3880			G3623		C	
					U3881			A3624		C	
					U3882			G3625		C	
					U3883			A3626		C	
					U3884			G3627		C	
					U3885			A3628		C	
					U3886			G3629		C	
					U3887			A3630		C	
					U3888			G3631		C	
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					U3896			G3639		C	
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					U3918			G3661		C	
					U3919			A3662		C	
					U3920			G3663		C	
					U3921			A3664		C	
					U3922			G3665		C	
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					U3924			G3667		C	
					U3925			A3668		C	
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					U3928			G3671		C	
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					U3930			G3673		C	
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					U3958			G3701		C	
					U3959			A3702		C	
					U3960			G3703		C	
					U3961			A3704		C	
					U3962			G3705		C	
					U3963			A3706		C	
					U3964			G3707		C	</



- Molecule 2: 5.8S rRNA



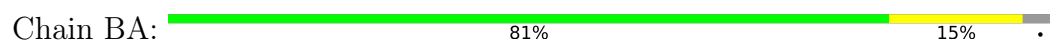
- Molecule 3: 5S rRNA



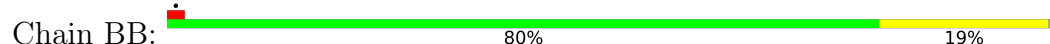
- Molecule 4: 60S ribosomal protein L41

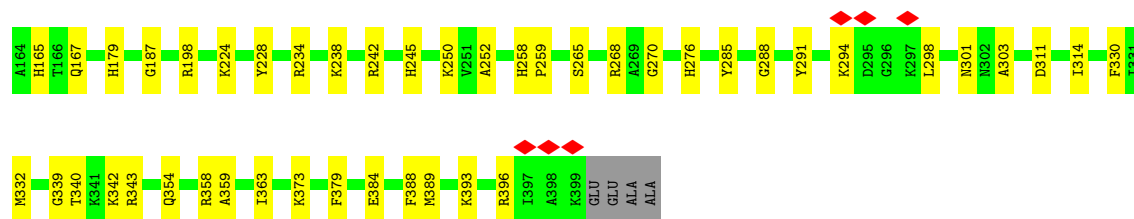


- Molecule 5: 60S ribosomal protein L8



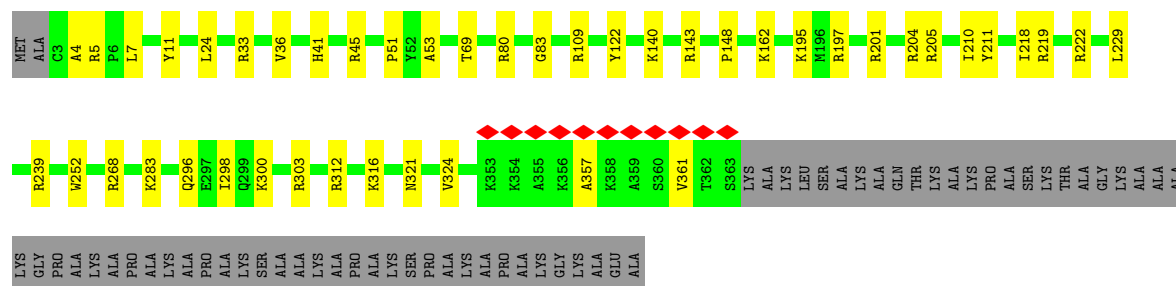
- Molecule 6: Ribosomal protein uL3





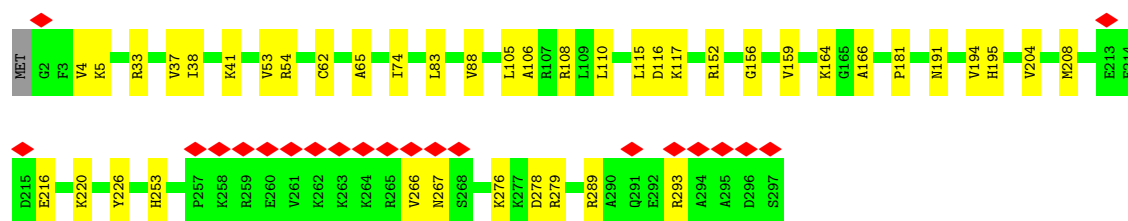
- Molecule 7: 60S ribosomal protein L4 C-terminal domain-containing protein

Chain BC: 75% 11% 14%



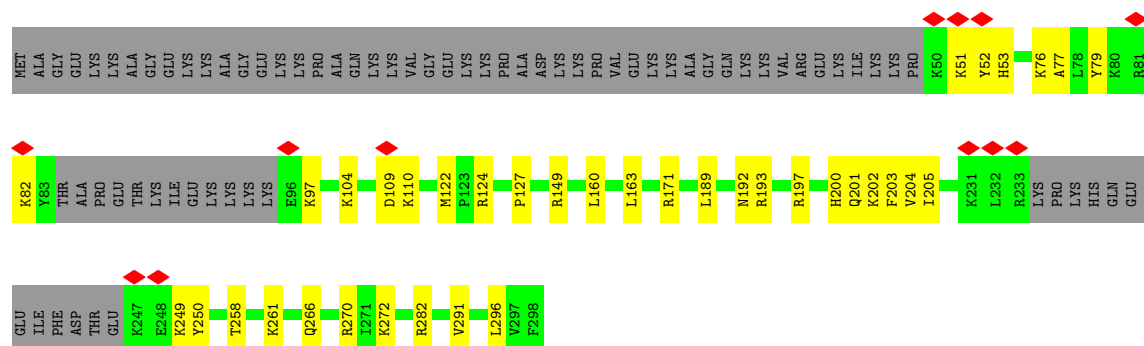
- Molecule 8: Large ribosomal subunit protein uL18

Chain BD: 86% 14% 7%



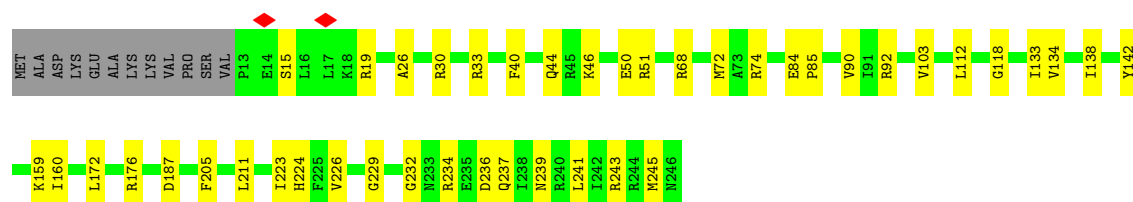
- Molecule 9: 60S ribosomal protein L6

Chain BE: 62% 13% 25%

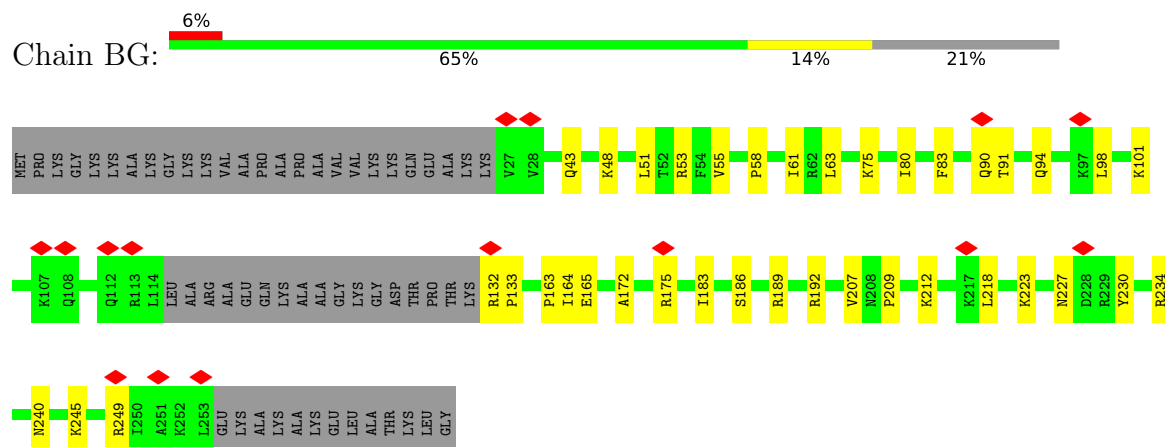


- Molecule 10: Large ribosomal subunit protein uL30

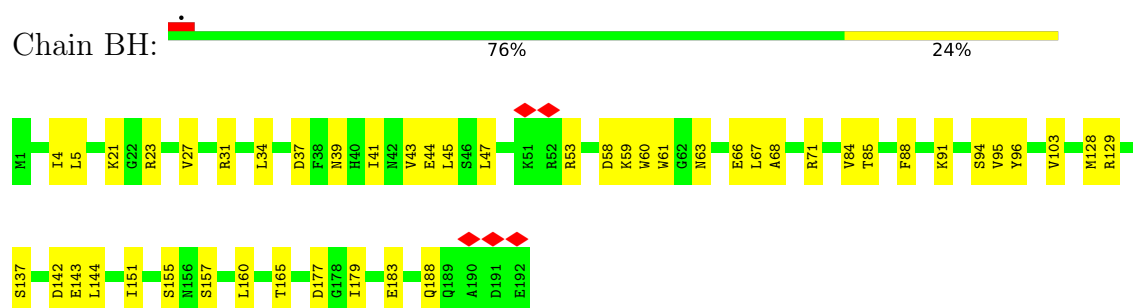
Chain BF: 78% 17% 5%



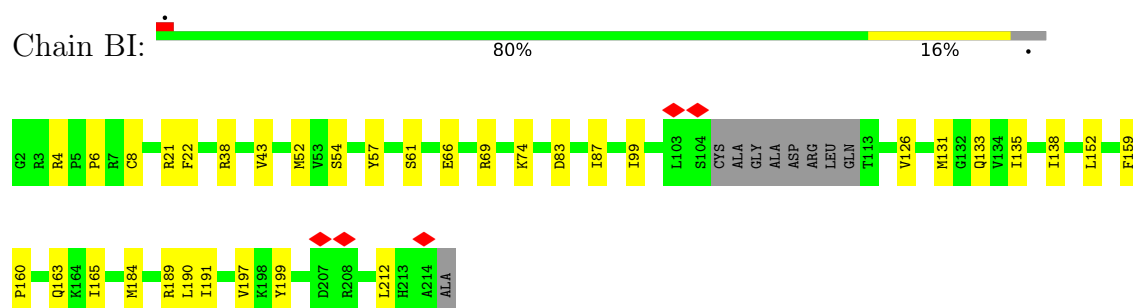
- Molecule 11: Large ribosomal subunit protein eL8



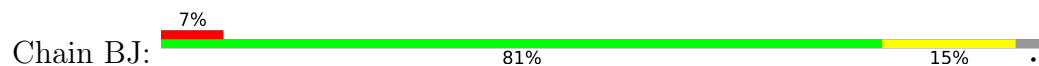
- Molecule 12: 60S ribosomal protein L9

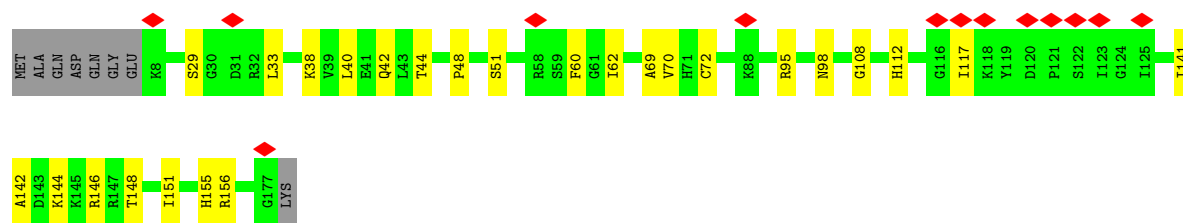


- Molecule 13: Large ribosomal subunit protein uL16

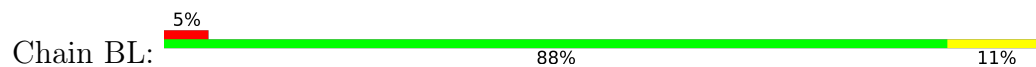


- Molecule 14: 60S ribosomal protein L11

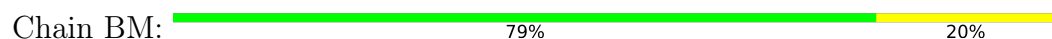




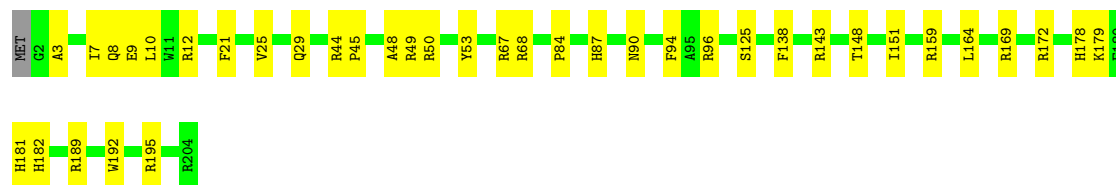
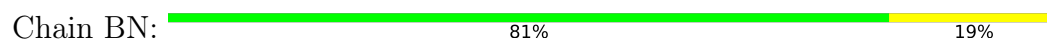
- Molecule 15: Large ribosomal subunit protein eL13



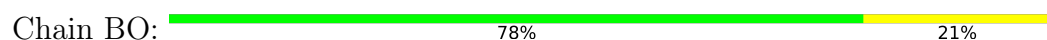
- Molecule 16: 60S ribosomal protein L14



- Molecule 17: Ribosomal protein L15



- Molecule 18: Ribosomal protein uL13



- Molecule 19: 60S ribosomal protein L17



LYS
LYS
LYS
ILE
SER
GLN
LYS
LYS
LEU
LYS
LYS
GLN
LYS
LEU
MET
ALA
ARG
GLU

• Molecule 20: Ribosomal protein L18

Chain BQ: 85% 15%

G2 K9 K12 K15 K19 D22 L35 R38 T39 N40 K49 R65 L72 R75 V82 A102 R112 R115 K132 R143 V148 K154 P159 T163 S169 K173 A177 R179 R184 R188

• Molecule 21: Ribosomal protein L19

Chain BR: 10% 80% 12% 8%

MET S2 N36 S37 Q40 K46 R60 I78 M96 M99 R104 L105 R108 Y109 R117 L138 M139 D157 E160 A161 R162 R163 S164 K165 T166 K167 E168 A169 R170 K171 R172 R173 E174 E175 R176 L177 Q178 A179 K180 K181 GLU GLU ILE ILE LYS THR LEU

SER
LYS
GLU
GLU
THR
LYS
LYS

• Molecule 22: 60S ribosomal protein L18a

Chain BS: 85% 15%

M1 G5 C16 L17 P18 T19 P20 K21 M30 F47 L51 M54 T71 R74 V75 K76 M93 R98 T101 G104 R111 H117 V142 R157 V158 R161 Q162 H163 K164 M173 T174 F175 F176

• Molecule 23: 60S ribosomal protein L21

Chain BT: 78% 21%

MET T2 K5 G6 R17 H22 L27 Y30 M31 R32 I33 Y34 K35 K36 K43 G51 H54 M66 V67 T68 Q69 H70 K78 R79 V80 K81 G82 K83 K87 R88 R92 I93 T96 K97 H98 Q107 R108 E111 K117 K120 E121 K122 G123

I124 W125 V126 K129 R136 L151 A160

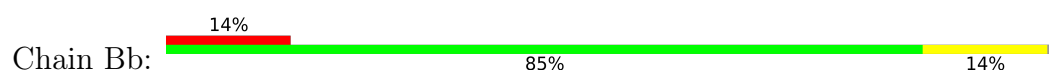
• Molecule 24: Large ribosomal subunit protein eL22

Chain BU: 10% 57% 21% 22%

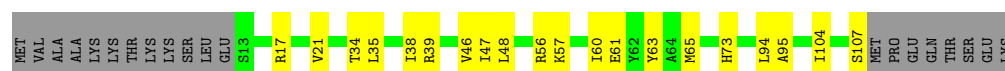
MET ALA PRO VAL LYS LYS PRO ALA ALA LYS GLY GLY LYS LYS LYS Q17 V18 L19 K20 F21 T22 L23 D24 D31 G32 I33 M34 Q35 F39 E40 K48 A53 G54 N55 G58 G59 V60 V61 S66 K67 S68 K69 V72 E75 K80 L83 K84 Y85 L86

T87 K88 K89 R97 D98 W99 V102 N105 Y110 E111 L112 R113 Q116 ILE ASN GLN ASP ASP GLU GLU GLU GLU GLU ASP

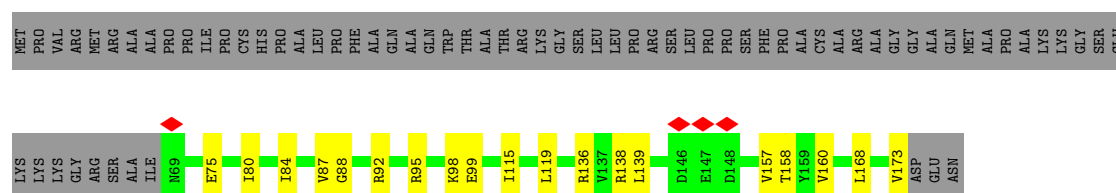
• Molecule 25: Large ribosomal subunit protein uL14



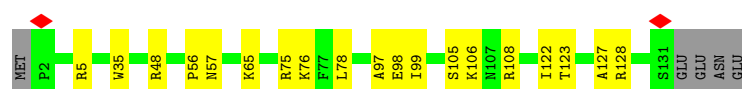
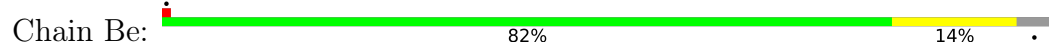
- Molecule 32: Large ribosomal subunit protein eL30



- Molecule 33: 60S ribosomal protein L31



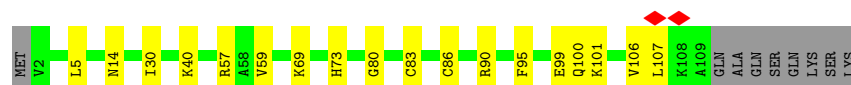
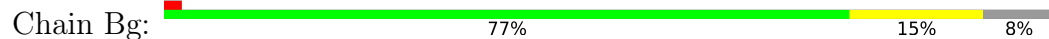
- Molecule 34: Ribosomal protein L32



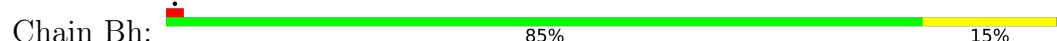
- Molecule 35: 60S ribosomal protein L35a



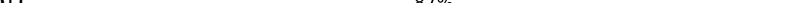
- Molecule 36: 60S ribosomal protein L34



- Molecule 37: Large ribosomal subunit protein uL29



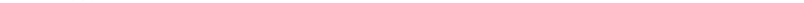


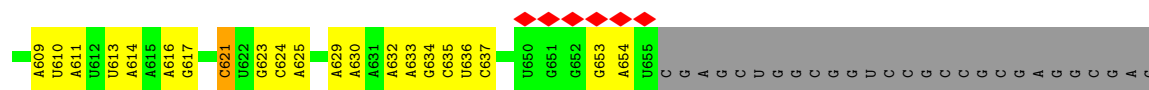
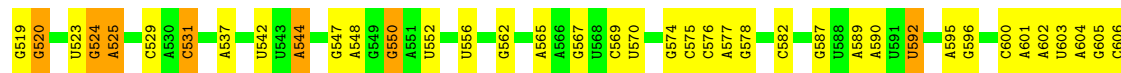
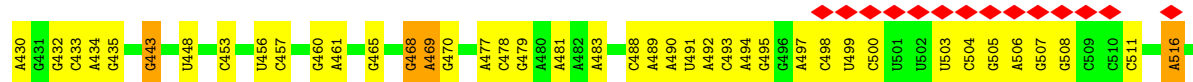
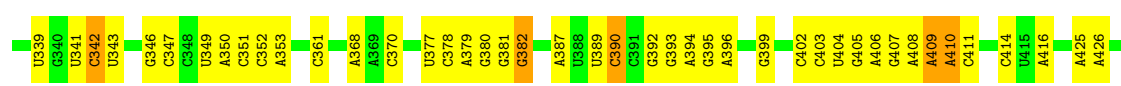
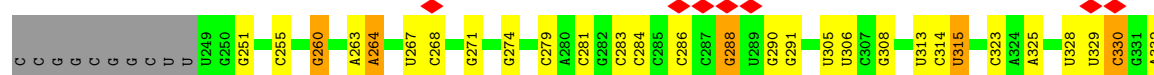
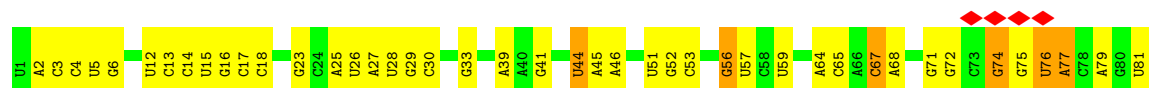
- Chain Bp:  87% 12%



- Chain Br:



- Chain A2: 





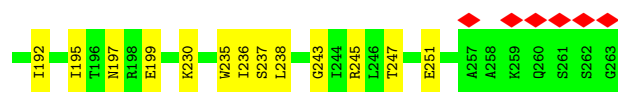
- Molecule 48: 40S ribosomal protein S27

- Molecule 49: 40S ribosomal protein S28

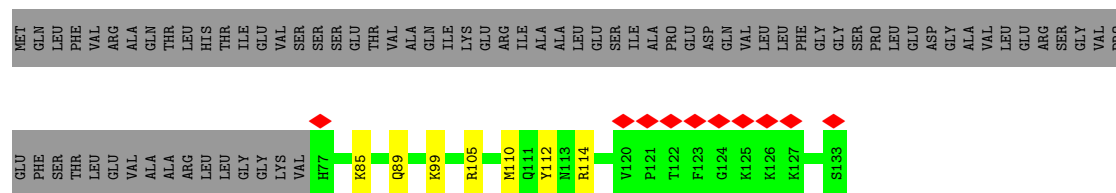
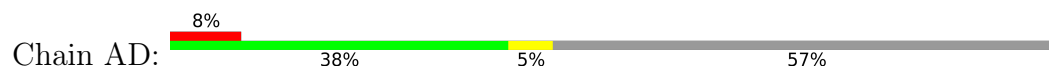
- Molecule 50: 40S ribosomal protein S2

- Molecule 51: Small ribosomal subunit protein eS4

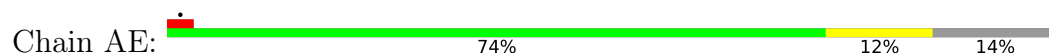




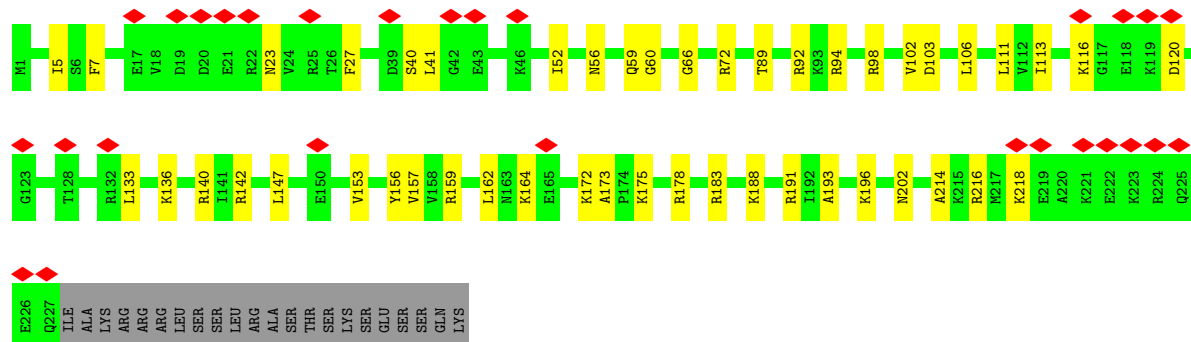
• Molecule 52: Ribosomal protein eS30



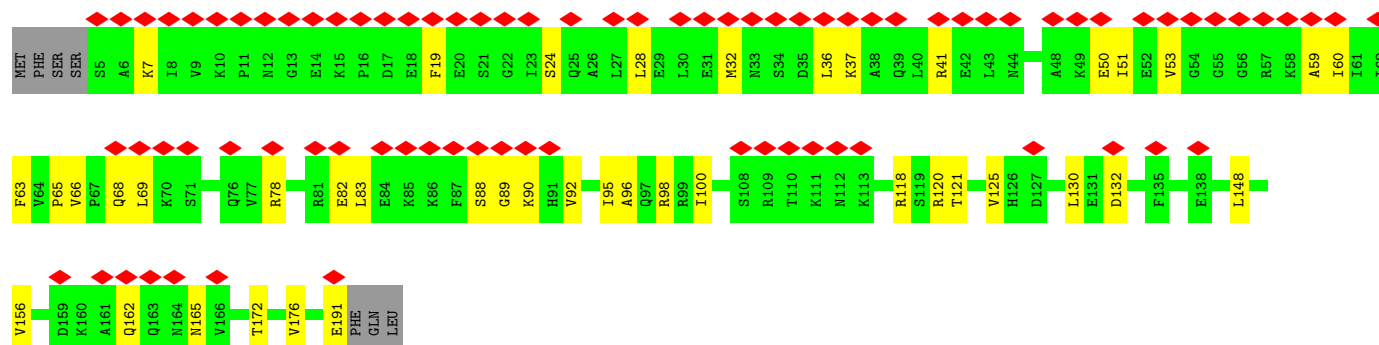
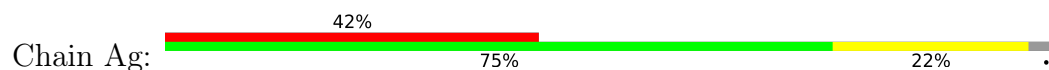
• Molecule 53: 40S ribosomal protein S26

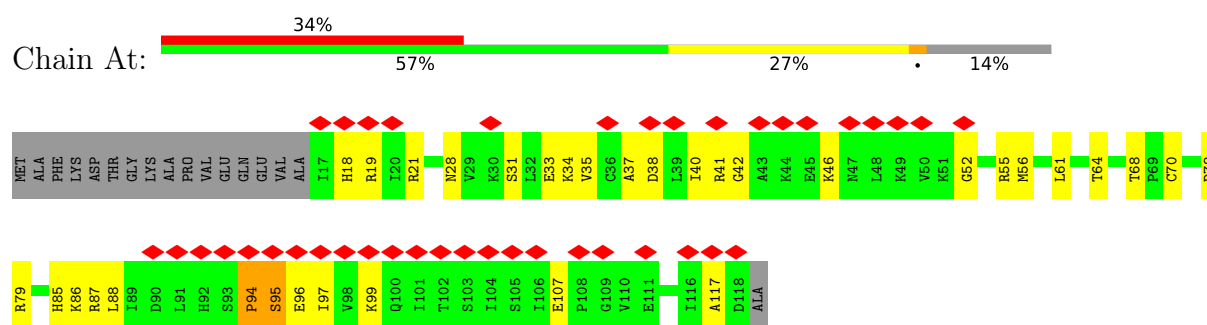


• Molecule 54: Small ribosomal subunit protein eS6

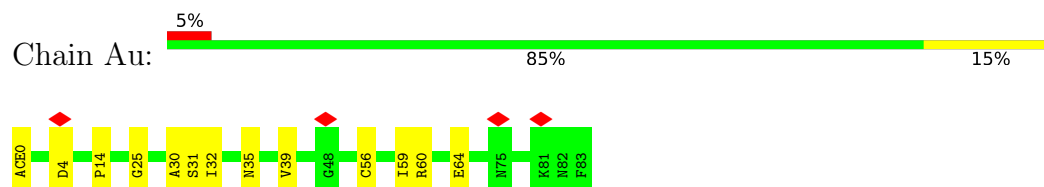


• Molecule 55: 40S ribosomal protein S7

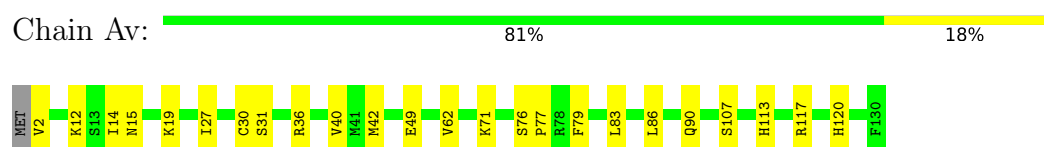




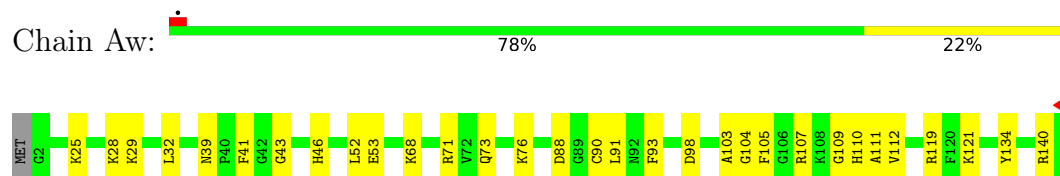
- Molecule 62: Small ribosomal subunit protein eS21



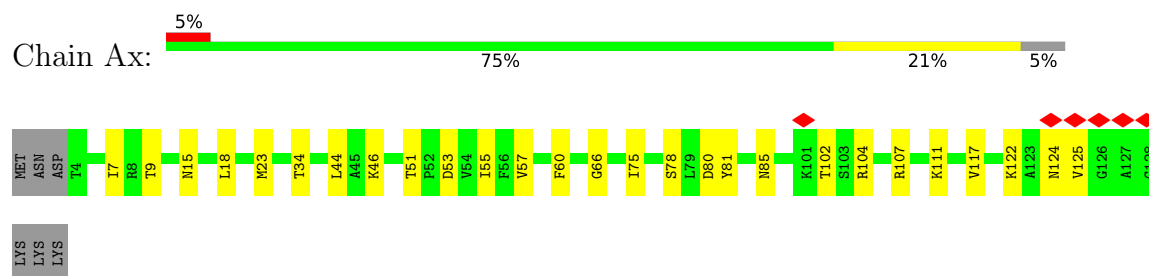
- Molecule 63: 40S ribosomal protein S15a



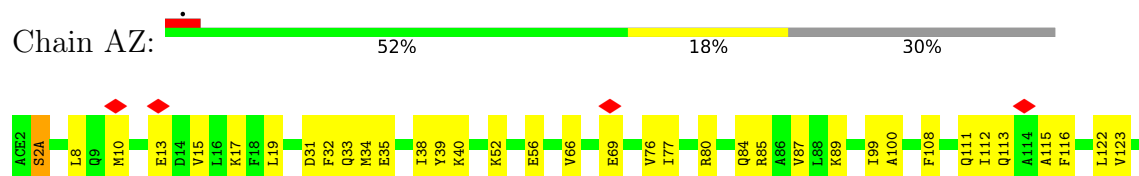
- Molecule 64: Small ribosomal subunit protein uS12

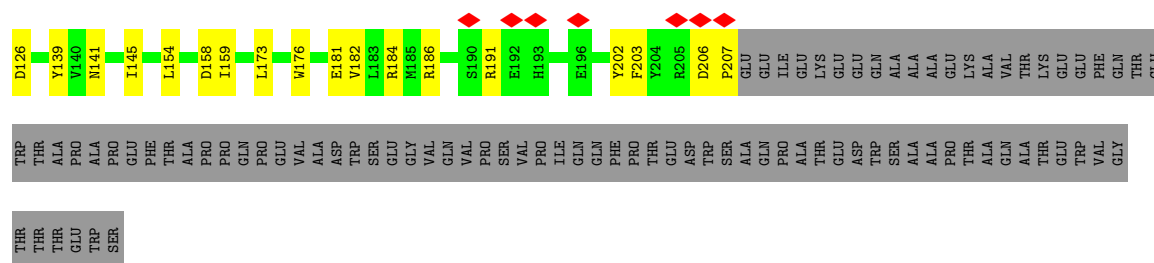


- Molecule 65: 40S ribosomal protein S24

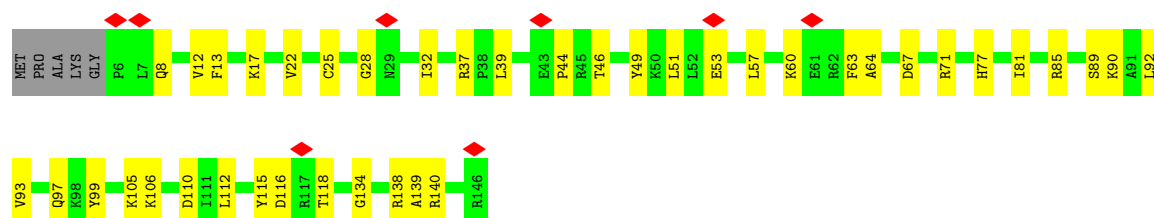
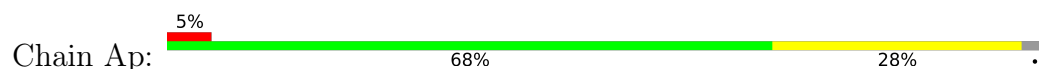


- Molecule 66: Small ribosomal subunit protein uS2

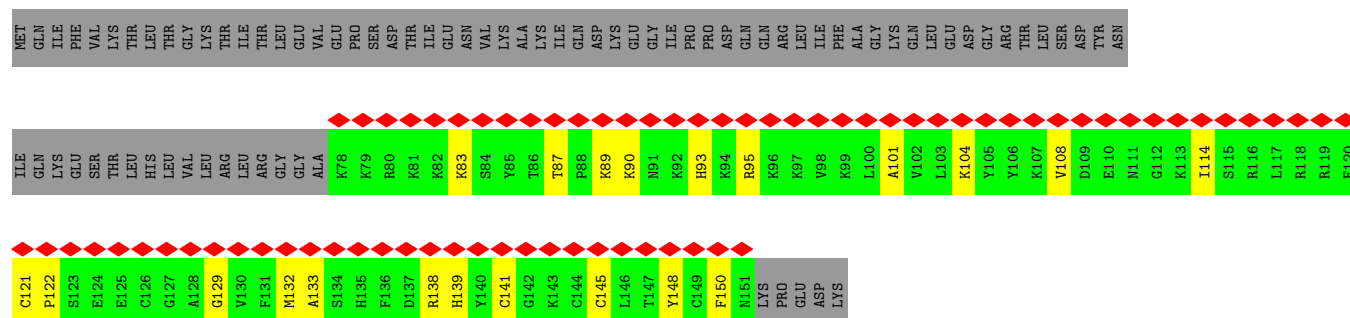
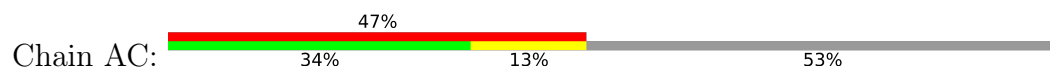




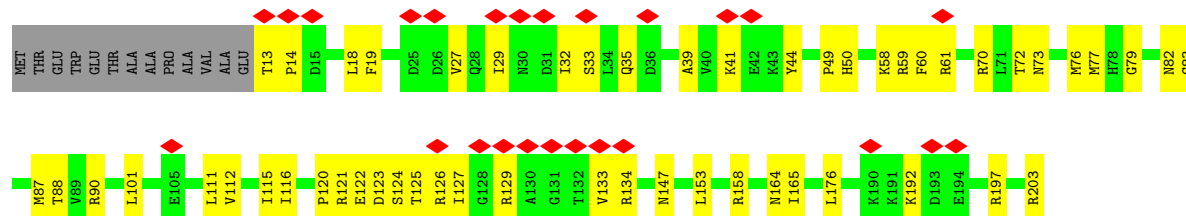
• Molecule 67: Ribosomal protein S16



• Molecule 68: Ubiquitin

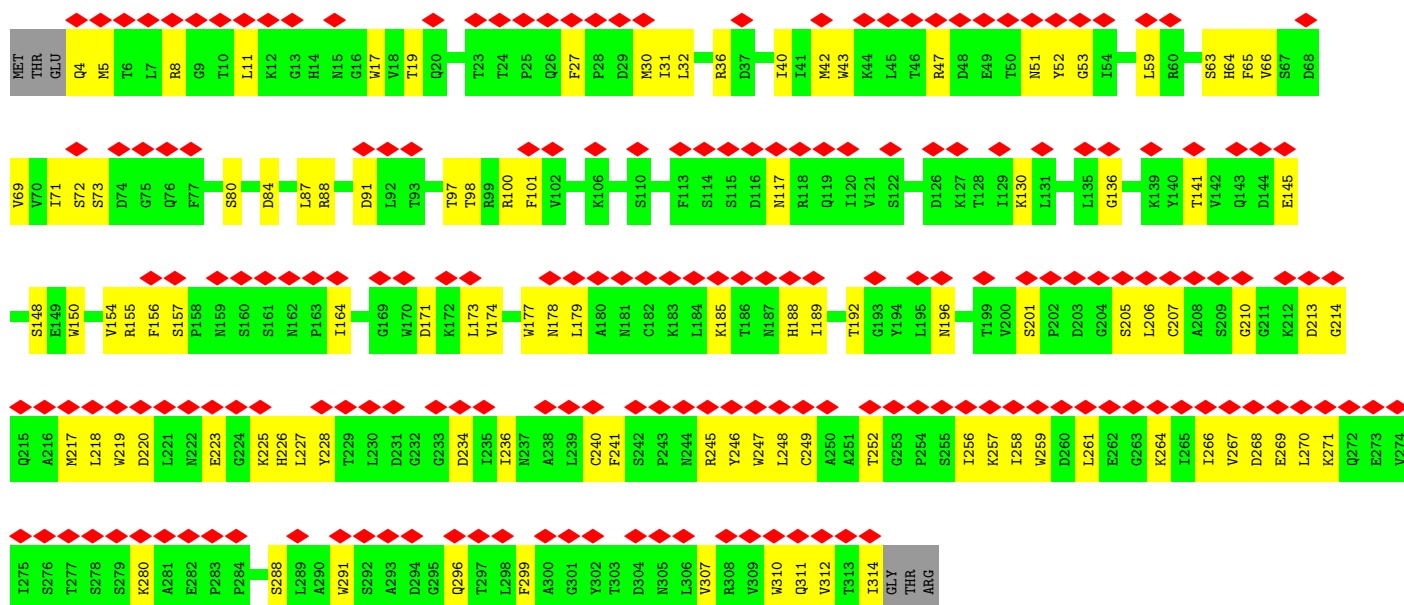


• Molecule 69: Ribosomal protein S5



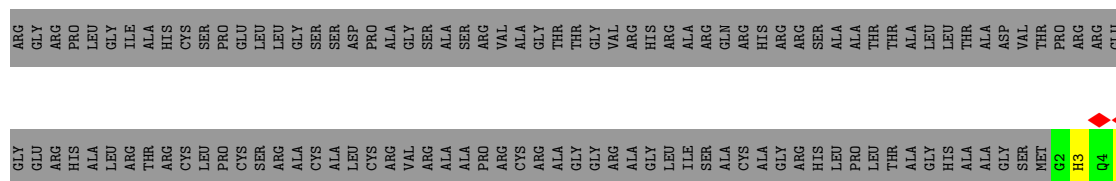
• Molecule 70: Small ribosomal subunit protein RACK1





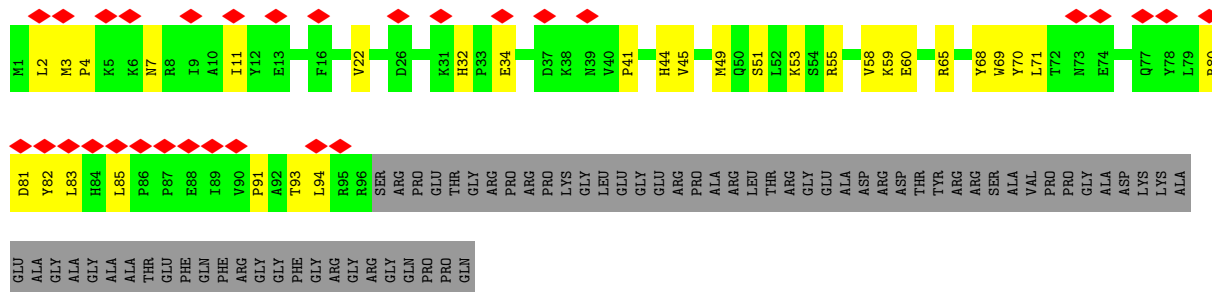
• Molecule 71: 40S ribosomal protein S29

Chain AG: 22% 10% 68%



• Molecule 72: Ribosomal protein S10

Chain Aj: 18% 39% 19% 42%

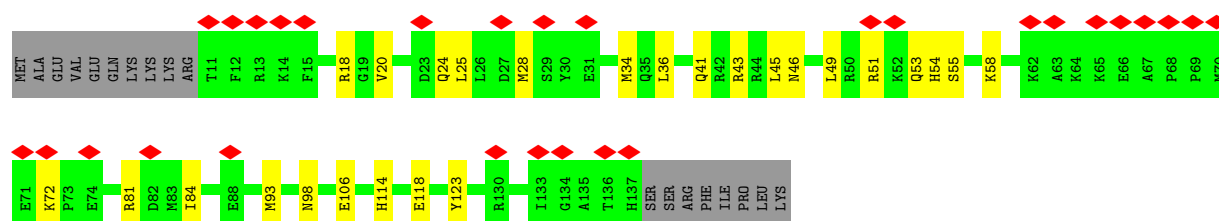
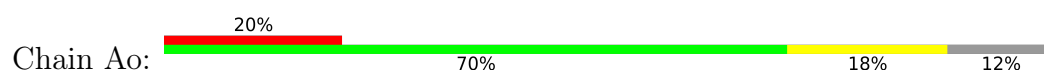


• Molecule 73: Small ribosomal subunit protein eS12

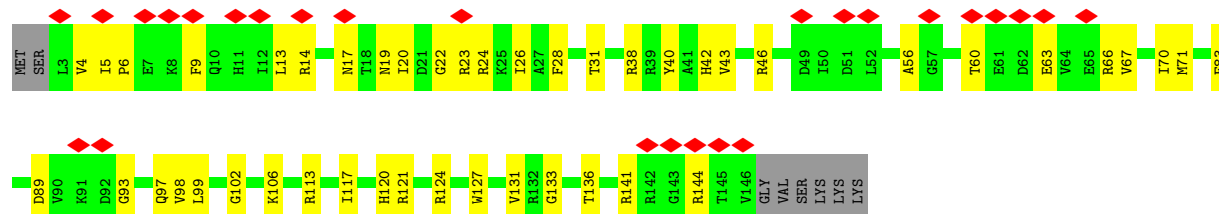
Chain Al: 89% 55% 34% 11%



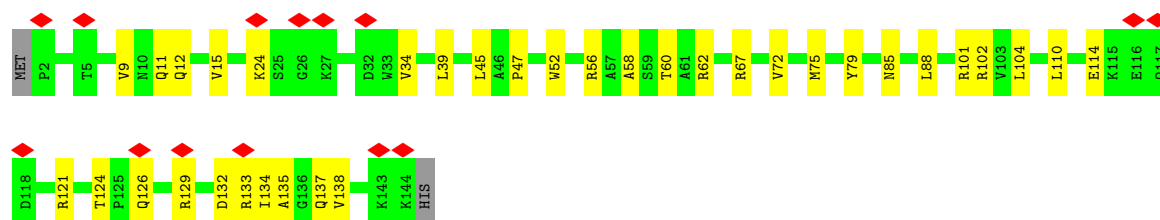
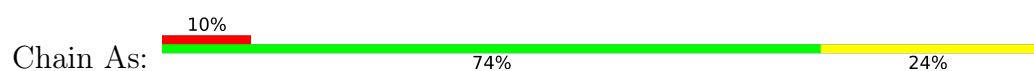
- Molecule 74: Small ribosomal subunit protein uS19



- Molecule 75: 40S ribosomal protein S18

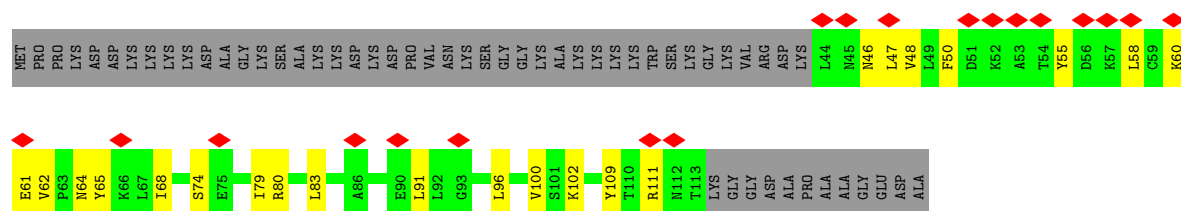


- Molecule 76: 40S ribosomal protein S19

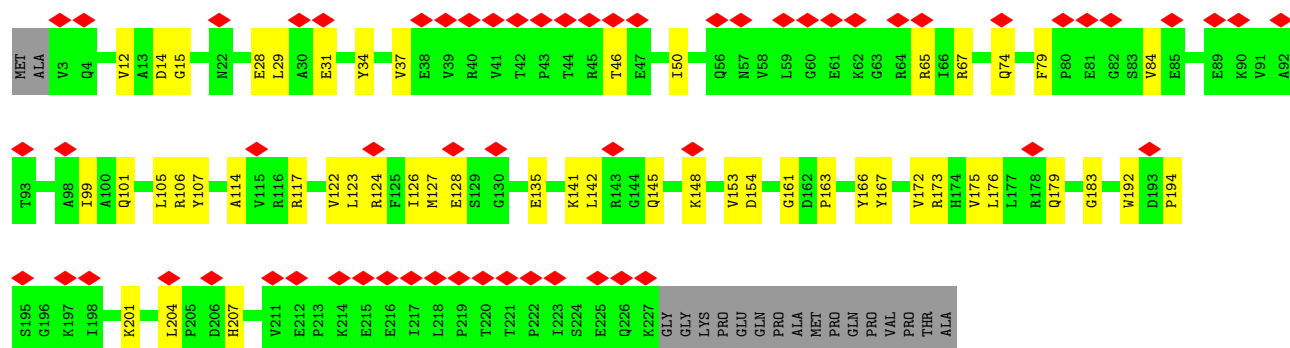
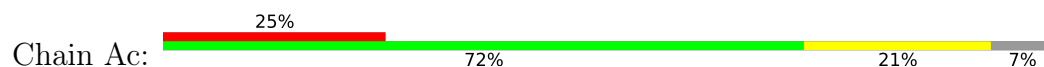


- Molecule 77: 40S ribosomal protein S25





• Molecule 78: DNA-(apurinic or apyrimidinic site) lyase



• Molecule 79: Phe tRNA



• Molecule 80: Small ribosomal subunit protein eS17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	122598	Depositor
Resolution determination method	FSC 3 SIGMA CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.826	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	465.74, 465.74, 465.74	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.803, 0.803, 0.803	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NMM, HIC, ZN, PSU, 6MZ, B8N, 4AC, OMU, MG, OMG, MA6, 1MA, UR3, IAS, MLZ, UY1, ACE, OMC, 5MC, A2M

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B5	0.15	0/83215	0.27	0/129832
2	B8	0.11	0/3656	0.24	0/5693
3	B7	0.12	0/2832	0.24	0/4413
4	Az	0.14	0/240	0.38	0/305
5	BA	0.14	0/1937	0.35	0/2597
6	BB	0.13	0/3264	0.31	0/4363
7	BC	0.13	0/2942	0.31	0/3950
8	BD	0.12	0/2431	0.31	0/3255
9	BE	0.11	0/1845	0.28	0/2466
10	BF	0.15	0/1975	0.34	0/2634
11	BG	0.13	0/1736	0.32	0/2342
12	BH	0.13	0/1552	0.30	0/2086
13	BI	0.13	0/1694	0.30	0/2264
14	BJ	0.12	0/1385	0.33	0/1852
15	BL	0.12	0/1742	0.30	0/2324
16	BM	0.13	0/1097	0.30	0/1460
17	BN	0.13	0/1745	0.29	0/2337
18	BO	0.14	0/1675	0.34	0/2239
19	BP	0.13	0/1285	0.33	0/1723
20	BQ	0.13	0/1527	0.31	0/2038
21	BR	0.14	0/1519	0.31	0/2007
22	BS	0.13	0/1503	0.32	0/2016
23	BT	0.13	0/1327	0.28	0/1771
24	BU	0.14	0/831	0.35	0/1115
25	BV	0.12	0/1007	0.32	0/1350
26	BW	0.12	0/573	0.32	0/763
27	BX	0.11	0/993	0.32	0/1334
28	BY	0.13	0/1123	0.33	0/1493
29	BZ	0.11	0/1130	0.24	0/1507
30	Ba	0.12	0/1209	0.30	0/1615
31	Bb	0.13	0/593	0.34	0/782

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Bc	0.12	0/748	0.29	0/1004
33	Bd	0.13	0/882	0.30	0/1187
34	Be	0.11	0/1093	0.27	0/1457
35	Bf	0.12	0/905	0.29	0/1211
36	Bg	0.12	0/870	0.32	0/1159
37	Bh	0.27	0/1023	0.35	0/1351
38	Bi	0.13	0/832	0.31	0/1100
39	Bj	0.13	0/718	0.35	0/948
40	Bk	0.12	0/575	0.31	0/761
41	Bl	0.12	0/452	0.26	0/596
42	Bm	0.10	0/435	0.29	0/575
43	Bo	0.12	0/864	0.29	0/1139
44	Bp	0.12	0/716	0.30	0/950
45	Br	0.14	0/1042	0.30	0/1398
46	A2	0.14	2/39049 (0.0%)	0.26	0/60848
47	Aa	0.12	0/1757	0.33	0/2352
48	AA	0.10	0/670	0.27	0/897
49	AB	0.11	0/508	0.31	0/680
50	Ab	0.12	0/1734	0.30	0/2342
51	Ad	0.11	0/2118	0.28	0/2848
52	AD	0.09	0/458	0.33	0/602
53	AE	0.12	0/806	0.31	0/1080
54	Af	0.11	0/1861	0.29	0/2481
55	Ag	0.12	0/1522	0.34	0/2039
56	Ah	0.12	0/1715	0.32	0/2289
57	Ai	0.13	0/1520	0.34	0/2030
58	Ak	0.12	0/1257	0.29	0/1680
59	Am	0.11	0/1232	0.25	0/1656
60	An	0.12	0/1020	0.34	0/1366
61	At	0.13	0/821	0.40	0/1103
62	Au	0.12	0/644	0.28	0/863
63	Av	0.13	0/1052	0.30	0/1408
64	Aw	0.19	0/1122	0.39	0/1498
65	Ax	0.11	0/1032	0.27	0/1371
66	AZ	0.14	0/1661	0.33	0/2259
67	Ap	0.13	0/1141	0.36	0/1527
68	AC	0.16	0/623	0.39	0/823
69	Ae	0.13	0/1531	0.37	0/2059
70	AF	0.12	0/2477	0.37	0/3372
71	AG	0.13	0/470	0.32	0/623
72	Aj	0.14	0/836	0.36	0/1128
73	Al	0.18	0/926	0.45	0/1244
74	Ao	0.11	0/1065	0.31	0/1424

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Ar	0.15	0/1209	0.38	0/1620
76	As	0.17	0/1120	0.36	0/1499
77	Ay	0.20	0/561	0.36	0/755
78	Ac	0.12	0/1780	0.32	0/2396
79	V	0.10	0/1822	0.25	0/2841
80	Aq	0.14	0/1095	0.35	0/1469
All	All	0.14	2/222953 (0.0%)	0.29	0/327234

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	A2	99	A2M	O3'-P	5.04	1.61	1.56
46	A2	1284	OMU	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B5	76444	0	38695	1072	0
2	B8	3338	0	1695	47	0
3	B7	2536	0	1284	24	0
4	Az	239	0	288	6	0
5	BA	1898	0	1995	30	0
6	BB	3209	0	3351	58	0
7	BC	2888	0	3057	46	0
8	BD	2388	0	2424	30	0
9	BE	1811	0	1973	28	0
10	BF	1939	0	2084	30	0
11	BG	1704	0	1821	32	0
12	BH	1533	0	1608	31	0
13	BI	1654	0	1703	24	0
14	BJ	1362	0	1398	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	BL	1710	0	1829	21	0
16	BM	1077	0	1140	23	0
17	BN	1700	0	1746	37	0
18	BO	1643	0	1787	41	0
19	BP	1259	0	1293	16	0
20	BQ	1503	0	1624	25	0
21	BR	1503	0	1656	22	0
22	BS	1464	0	1512	19	0
23	BT	1299	0	1370	29	0
24	BU	817	0	839	22	0
25	BV	993	0	1050	17	0
26	BW	560	0	569	10	0
27	BX	976	0	1053	10	0
28	BY	1106	0	1192	19	0
29	BZ	1107	0	1182	13	0
30	Ba	1179	0	1225	23	0
31	Bb	582	0	614	8	0
32	Bc	738	0	774	14	0
33	Bd	867	0	917	13	0
34	Be	1074	0	1174	15	0
35	Bf	886	0	924	9	0
36	Bg	860	0	955	15	0
37	Bh	1015	0	1148	12	0
38	Bi	821	0	903	13	0
39	Bj	704	0	738	9	0
40	Bk	569	0	637	9	0
41	Bl	442	0	483	6	0
42	Bm	429	0	465	6	0
43	Bo	861	0	930	9	0
44	Bp	706	0	756	8	0
45	Br	1025	0	1087	21	0
46	A2	35806	0	18114	544	0
47	Aa	1730	0	1803	39	0
48	AA	657	0	678	11	0
49	AB	506	0	536	13	0
50	Ab	1698	0	1788	40	0
51	Ad	2076	0	2176	33	0
52	AD	452	0	494	5	0
53	AE	793	0	841	11	0
54	Af	1838	0	1973	33	0
55	Ag	1500	0	1602	28	0
56	Ah	1685	0	1772	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	Ai	1495	0	1615	28	0
58	Ak	1236	0	1306	16	0
59	Am	1208	0	1294	17	0
60	An	1016	0	1038	29	0
61	At	811	0	877	25	0
62	Au	640	0	643	11	0
63	Av	1035	0	1080	22	0
64	Aw	1104	0	1172	20	0
65	Ax	1015	0	1086	19	0
66	AZ	1626	0	1636	41	0
67	Ap	1123	0	1193	29	0
68	AC	611	0	637	21	0
69	Ae	1509	0	1563	43	0
70	AF	2420	0	2380	78	0
71	AG	459	0	448	15	0
72	Aj	812	0	840	22	0
73	Al	916	0	943	38	0
74	Ao	1044	0	1089	21	0
75	Ar	1191	0	1253	33	0
76	As	1115	0	1147	29	0
77	Ay	555	0	608	19	0
78	Ac	1752	0	1848	33	0
79	V	1628	0	826	28	0
80	Aq	1081	0	1138	46	0
81	A2	104	0	0	0	0
81	Ak	1	0	0	0	0
81	An	3	0	0	0	0
81	As	1	0	0	0	0
81	B5	346	0	0	0	0
81	B7	11	0	0	0	0
81	B8	9	0	0	0	0
81	BA	3	0	0	0	0
81	BH	1	0	0	0	0
81	BI	2	0	0	0	0
81	BN	2	0	0	0	0
81	BP	2	0	0	0	0
81	BV	1	0	0	0	0
81	Ba	1	0	0	0	0
81	Bb	2	0	0	0	0
81	Be	1	0	0	0	0
81	Bf	1	0	0	0	0
81	Bg	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	Bj	1	0	0	0	0
81	Bo	1	0	0	0	0
82	AE	1	0	0	0	0
82	AG	1	0	0	0	0
82	Bg	1	0	0	0	0
82	Bj	1	0	0	0	0
82	Bm	1	0	0	0	0
82	Bo	1	0	0	0	0
82	Bp	1	0	0	0	0
83	A2	832	0	0	5	0
83	AA	8	0	0	0	0
83	AB	1	0	0	0	0
83	AD	2	0	0	0	0
83	AE	9	0	0	0	0
83	AG	2	0	0	1	0
83	AZ	3	0	0	0	0
83	Aa	10	0	0	0	0
83	Ab	11	0	0	0	0
83	Ad	10	0	0	0	0
83	Ae	2	0	0	0	0
83	Af	1	0	0	0	0
83	Ah	7	0	0	0	0
83	Ai	7	0	0	0	0
83	Ak	10	0	0	0	0
83	Am	4	0	0	0	0
83	An	7	0	0	0	0
83	Ap	1	0	0	0	0
83	Aq	4	0	0	0	0
83	Ar	1	0	0	0	0
83	At	3	0	0	0	0
83	Au	2	0	0	0	0
83	Av	10	0	0	0	0
83	Aw	8	0	0	0	0
83	Ax	4	0	0	0	0
83	Ay	4	0	0	0	0
83	Az	5	0	0	0	0
83	B5	4198	0	0	11	0
83	B7	30	0	0	1	0
83	B8	72	0	0	0	0
83	BA	28	0	0	1	0
83	BB	49	0	0	2	0
83	BC	45	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	BD	22	0	0	1	0
83	BE	11	0	0	0	0
83	BF	24	0	0	0	0
83	BG	15	0	0	1	0
83	BH	15	0	0	0	0
83	BI	13	0	0	0	0
83	BJ	3	0	0	0	0
83	BL	29	0	0	0	0
83	BM	6	0	0	0	0
83	BN	29	0	0	1	0
83	BO	19	0	0	0	0
83	BP	23	0	0	0	0
83	BQ	24	0	0	0	0
83	BR	9	0	0	0	0
83	BS	21	0	0	0	0
83	BT	21	0	0	0	0
83	BU	2	0	0	1	0
83	BV	17	0	0	1	0
83	BW	4	0	0	1	0
83	BX	5	0	0	0	0
83	BY	11	0	0	0	0
83	BZ	5	0	0	0	0
83	Ba	23	0	0	1	0
83	Bb	11	0	0	0	0
83	Bc	5	0	0	0	0
83	Bd	9	0	0	0	0
83	Be	17	0	0	0	0
83	Bf	25	0	0	0	0
83	Bg	9	0	0	0	0
83	Bh	3	0	0	0	0
83	Bi	8	0	0	1	0
83	Bj	16	0	0	0	0
83	Bl	5	0	0	0	0
83	Bm	5	0	0	1	0
83	Bo	15	0	0	0	0
83	Bp	12	0	0	0	0
83	Br	16	0	0	1	0
83	V	9	0	0	0	0
All	All	216968	0	156385	2924	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2924 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B5:1669:G:H1	1:B5:1679:U:H3	1.04	0.99
1:B5:449:G:H3'	1:B5:450:C:H4'	1.48	0.93
80:Aq:31:ASN:HD22	80:Aq:55:THR:HG22	1.36	0.91
70:AF:173:LEU:HD22	70:AF:189:ILE:HG22	1.52	0.91
76:As:126:GLN:O	76:As:129:ARG:NH1	2.03	0.91

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Az	23/25 (92%)	23 (100%)	0	0	100	100
5	BA	246/257 (96%)	238 (97%)	8 (3%)	0	100	100
6	BB	395/403 (98%)	388 (98%)	7 (2%)	0	100	100
7	BC	359/421 (85%)	353 (98%)	6 (2%)	0	100	100
8	BD	294/297 (99%)	284 (97%)	10 (3%)	0	100	100
9	BE	218/298 (73%)	215 (99%)	3 (1%)	0	100	100
10	BF	232/246 (94%)	225 (97%)	7 (3%)	0	100	100
11	BG	206/266 (77%)	201 (98%)	5 (2%)	0	100	100
12	BH	190/192 (99%)	190 (100%)	0	0	100	100
13	BI	201/214 (94%)	197 (98%)	4 (2%)	0	100	100
14	BJ	168/178 (94%)	165 (98%)	3 (2%)	0	100	100
15	BL	208/211 (99%)	202 (97%)	5 (2%)	1 (0%)	24	43
16	BM	128/131 (98%)	126 (98%)	2 (2%)	0	100	100
17	BN	201/204 (98%)	196 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	BO	199/203 (98%)	196 (98%)	3 (2%)	0	100	100
19	BP	153/184 (83%)	151 (99%)	2 (1%)	0	100	100
20	BQ	185/187 (99%)	183 (99%)	2 (1%)	0	100	100
21	BR	178/196 (91%)	177 (99%)	1 (1%)	0	100	100
22	BS	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
23	BT	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	BU	98/128 (77%)	94 (96%)	4 (4%)	0	100	100
25	BV	132/140 (94%)	131 (99%)	1 (1%)	0	100	100
26	BW	65/157 (41%)	65 (100%)	0	0	100	100
27	BX	117/155 (76%)	113 (97%)	4 (3%)	0	100	100
28	BY	131/145 (90%)	129 (98%)	2 (2%)	0	100	100
29	BZ	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
30	Ba	145/148 (98%)	142 (98%)	3 (2%)	0	100	100
31	Bb	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
32	Bc	93/115 (81%)	93 (100%)	0	0	100	100
33	Bd	103/176 (58%)	101 (98%)	2 (2%)	0	100	100
34	Be	128/135 (95%)	126 (98%)	2 (2%)	0	100	100
35	Bf	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
36	Bg	106/117 (91%)	105 (99%)	1 (1%)	0	100	100
37	Bh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
38	Bi	98/105 (93%)	96 (98%)	2 (2%)	0	100	100
39	Bj	84/97 (87%)	84 (100%)	0	0	100	100
40	Bk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
41	Bl	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
42	Bm	50/128 (39%)	50 (100%)	0	0	100	100
43	Bo	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
44	Bp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Br	124/138 (90%)	121 (98%)	3 (2%)	0	100	100
47	Aa	211/264 (80%)	207 (98%)	4 (2%)	0	100	100
48	AA	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
49	AB	62/69 (90%)	59 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	Ab	217/264 (82%)	215 (99%)	2 (1%)	0	100	100
51	Ad	260/263 (99%)	254 (98%)	6 (2%)	0	100	100
52	AD	55/133 (41%)	53 (96%)	2 (4%)	0	100	100
53	AE	97/115 (84%)	96 (99%)	1 (1%)	0	100	100
54	Af	225/249 (90%)	224 (100%)	1 (0%)	0	100	100
55	Ag	185/194 (95%)	175 (95%)	10 (5%)	0	100	100
56	Ah	204/207 (99%)	193 (95%)	11 (5%)	0	100	100
57	Ai	177/194 (91%)	173 (98%)	3 (2%)	1 (1%)	21	38
58	Ak	150/158 (95%)	147 (98%)	3 (2%)	0	100	100
59	Am	148/151 (98%)	148 (100%)	0	0	100	100
60	An	132/151 (87%)	122 (92%)	10 (8%)	0	100	100
61	At	100/119 (84%)	85 (85%)	13 (13%)	2 (2%)	6	10
62	Au	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
63	Av	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
64	Aw	140/143 (98%)	134 (96%)	6 (4%)	0	100	100
65	Ax	123/131 (94%)	123 (100%)	0	0	100	100
66	AZ	205/296 (69%)	198 (97%)	7 (3%)	0	100	100
67	Ap	139/146 (95%)	128 (92%)	11 (8%)	0	100	100
68	AC	72/156 (46%)	62 (86%)	10 (14%)	0	100	100
69	Ae	189/204 (93%)	179 (95%)	10 (5%)	0	100	100
70	AF	309/317 (98%)	288 (93%)	21 (7%)	0	100	100
71	AG	53/171 (31%)	52 (98%)	1 (2%)	0	100	100
72	Aj	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
73	Al	116/132 (88%)	102 (88%)	14 (12%)	0	100	100
74	Ao	125/145 (86%)	118 (94%)	7 (6%)	0	100	100
75	Ar	142/152 (93%)	131 (92%)	11 (8%)	0	100	100
76	As	140/145 (97%)	136 (97%)	4 (3%)	0	100	100
77	Ay	68/125 (54%)	68 (100%)	0	0	100	100
78	Ac	223/243 (92%)	221 (99%)	2 (1%)	0	100	100
80	Aq	132/135 (98%)	122 (92%)	10 (8%)	0	100	100
All	All	11107/12726 (87%)	10791 (97%)	312 (3%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BL	64	VAL
57	Ai	139	LYS
61	At	95	SER
61	At	94	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Az	24/24 (100%)	24 (100%)	0	100	100
5	BA	190/199 (96%)	190 (100%)	0	100	100
6	BB	346/349 (99%)	346 (100%)	0	100	100
7	BC	305/338 (90%)	305 (100%)	0	100	100
8	BD	248/249 (100%)	248 (100%)	0	100	100
9	BE	195/256 (76%)	195 (100%)	0	100	100
10	BF	201/211 (95%)	201 (100%)	0	100	100
11	BG	186/225 (83%)	185 (100%)	1 (0%)	81	92
12	BH	171/171 (100%)	171 (100%)	0	100	100
13	BI	173/178 (97%)	173 (100%)	0	100	100
14	BJ	142/148 (96%)	142 (100%)	0	100	100
15	BL	177/178 (99%)	177 (100%)	0	100	100
16	BM	112/113 (99%)	112 (100%)	0	100	100
17	BN	171/172 (99%)	171 (100%)	0	100	100
18	BO	172/173 (99%)	172 (100%)	0	100	100
19	BP	136/163 (83%)	135 (99%)	1 (1%)	76	89
20	BQ	159/159 (100%)	159 (100%)	0	100	100
21	BR	159/175 (91%)	159 (100%)	0	100	100
22	BS	157/157 (100%)	157 (100%)	0	100	100
23	BT	139/140 (99%)	139 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BU	90/113 (80%)	90 (100%)	0	100	100
25	BV	102/107 (95%)	102 (100%)	0	100	100
26	BW	59/127 (46%)	59 (100%)	0	100	100
27	BX	107/134 (80%)	107 (100%)	0	100	100
28	BY	123/135 (91%)	123 (100%)	0	100	100
29	BZ	117/118 (99%)	117 (100%)	0	100	100
30	Ba	121/122 (99%)	121 (100%)	0	100	100
31	Bb	61/62 (98%)	61 (100%)	0	100	100
32	Bc	80/98 (82%)	80 (100%)	0	100	100
33	Bd	95/148 (64%)	95 (100%)	0	100	100
34	Be	118/123 (96%)	118 (100%)	0	100	100
35	Bf	89/89 (100%)	89 (100%)	0	100	100
36	Bg	93/101 (92%)	93 (100%)	0	100	100
37	Bh	109/110 (99%)	109 (100%)	0	100	100
38	Bi	85/89 (96%)	85 (100%)	0	100	100
39	Bj	73/80 (91%)	73 (100%)	0	100	100
40	Bk	64/65 (98%)	64 (100%)	0	100	100
41	Bl	47/48 (98%)	47 (100%)	0	100	100
42	Bm	48/115 (42%)	48 (100%)	0	100	100
43	Bo	92/92 (100%)	92 (100%)	0	100	100
44	Bp	74/75 (99%)	74 (100%)	0	100	100
45	Br	111/118 (94%)	111 (100%)	0	100	100
47	Aa	194/228 (85%)	194 (100%)	0	100	100
48	AA	75/76 (99%)	75 (100%)	0	100	100
49	AB	57/62 (92%)	57 (100%)	0	100	100
50	Ab	185/214 (86%)	185 (100%)	0	100	100
51	Ad	223/224 (100%)	223 (100%)	0	100	100
52	AD	46/108 (43%)	46 (100%)	0	100	100
53	AE	87/99 (88%)	87 (100%)	0	100	100
54	Af	199/219 (91%)	199 (100%)	0	100	100
55	Ag	167/174 (96%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	Ah	177/178 (99%)	177 (100%)	0	100	100
57	Ai	160/168 (95%)	160 (100%)	0	100	100
58	Ak	135/140 (96%)	135 (100%)	0	100	100
59	Am	130/131 (99%)	130 (100%)	0	100	100
60	An	105/118 (89%)	105 (100%)	0	100	100
61	At	94/106 (89%)	94 (100%)	0	100	100
62	Au	69/69 (100%)	69 (100%)	0	100	100
63	Av	112/113 (99%)	112 (100%)	0	100	100
64	Aw	114/115 (99%)	114 (100%)	0	100	100
65	Ax	107/113 (95%)	107 (100%)	0	100	100
66	AZ	172/245 (70%)	171 (99%)	1 (1%)	78	91
67	Ap	116/119 (98%)	116 (100%)	0	100	100
68	AC	67/140 (48%)	67 (100%)	0	100	100
69	Ae	161/170 (95%)	161 (100%)	0	100	100
70	AF	270/275 (98%)	270 (100%)	0	100	100
71	AG	48/130 (37%)	48 (100%)	0	100	100
72	Aj	88/136 (65%)	88 (100%)	0	100	100
73	Al	100/109 (92%)	100 (100%)	0	100	100
74	Ao	113/130 (87%)	113 (100%)	0	100	100
75	Ar	125/132 (95%)	125 (100%)	0	100	100
76	As	112/114 (98%)	112 (100%)	0	100	100
77	Ay	61/102 (60%)	61 (100%)	0	100	100
78	Ac	189/202 (94%)	189 (100%)	0	100	100
80	Aq	120/121 (99%)	120 (100%)	0	100	100
All	All	9699/10827 (90%)	9696 (100%)	3 (0%)	100	100

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	BG	90	GLN
19	BP	93	HIS
66	AZ	2(A)	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106

such sidechains are listed below:

Mol	Chain	Res	Type
41	B1	17	GLN
53	AE	25	ASN
74	Ao	35	GLN
42	Bm	84	GLN
49	AB	29	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B5	3554/4441 (80%)	559 (15%)	23 (0%)
2	B8	156/157 (99%)	16 (10%)	0
3	B7	118/119 (99%)	8 (6%)	0
46	A2	1670/1823 (91%)	297 (17%)	3 (0%)
79	V	75/76 (98%)	26 (34%)	1 (1%)
All	All	5573/6616 (84%)	906 (16%)	27 (0%)

5 of 906 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B5	39	A
1	B5	42	A
1	B5	58	G
1	B5	59	A
1	B5	64	A

5 of 27 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B5	2005	G
1	B5	3249	U
46	A2	1733	G
1	B5	3245	U
1	B5	4142	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

142 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	B5	3736	1	18,21,22	0.49	0	22,30,33	0.55	0
1	PSU	B5	1771	1	18,21,22	0.47	0	22,30,33	0.61	0
1	A2M	B5	3195	1	22,25,26	0.09	0	31,36,39	0.21	0
1	PSU	B5	1600	1	18,21,22	0.66	1 (5%)	22,30,33	0.59	0
1	OMG	B5	3813	1	23,26,27	0.28	0	33,38,41	0.39	0
1	PSU	B5	4071	1	18,21,22	0.51	0	22,30,33	0.57	0
60	IAS	An	138	60	6,7,8	1.05	0	6,8,10	1.30	1 (16%)
1	PSU	B5	3397	1,81	18,21,22	0.47	0	22,30,33	0.59	0
1	PSU	B5	1769	1	18,21,22	0.49	0	22,30,33	0.57	0
1	OMG	B5	3376	1,81	23,26,27	0.31	0	33,38,41	0.49	0
1	A2M	B5	1251	1	22,25,26	0.07	0	31,36,39	0.23	0
1	PSU	B5	3874	1	18,21,22	0.47	0	22,30,33	0.60	0
1	PSU	B5	3192	1	18,21,22	0.54	0	22,30,33	0.59	1 (4%)
1	OMG	B5	4080	1	23,26,27	0.29	0	33,38,41	0.35	0
1	A2M	B5	2564	1	22,25,26	0.08	0	31,36,39	0.20	0
46	OMG	A2	605	46	23,26,27	0.28	0	33,38,41	0.44	0
1	OMC	B5	3979	1	19,22,23	0.32	0	26,31,34	0.47	0
2	OMG	B8	75	2	23,26,27	0.29	0	33,38,41	0.39	0
46	OMU	A2	315	46	19,22,23	0.33	0	26,31,34	0.64	0
1	5MC	B5	3259	1,81	18,22,23	0.29	0	26,32,35	0.43	0
1	PSU	B5	3739	1	18,21,22	0.47	0	22,30,33	0.62	0
6	HIC	BB	245	6	10,11,12	1.55	2 (20%)	8,14,16	0.97	0
1	1MA	B5	1247	1,81	21,25,26	0.30	0	31,37,40	0.46	0
1	PSU	B5	3975	1	18,21,22	0.52	0	22,30,33	0.55	0
1	PSU	B5	3846	1	18,21,22	0.49	0	22,30,33	0.58	0
1	A2M	B5	3201	1	22,25,26	0.07	0	31,36,39	0.18	0
46	MA6	A2	1804	46	23,26,27	0.32	0	34,38,41	0.66	1 (2%)
46	A2M	A2	989	46	22,25,26	0.08	0	31,36,39	0.35	0
1	5MC	B5	3890	1	18,22,23	0.34	0	26,32,35	0.63	0
46	PSU	A2	774	46	18,21,22	0.47	0	22,30,33	0.60	0
1	OMC	B5	3178	1,81	19,22,23	0.26	0	26,31,34	0.47	0
46	A2M	A2	1341	46	22,25,26	0.09	0	31,36,39	0.23	0
46	B8N	A2	1206	46	24,29,30	0.58	0	29,42,45	0.64	0
1	PSU	B5	1690	1	18,21,22	0.47	0	22,30,33	0.59	0
46	6MZ	A2	1786	46,81	22,25,26	0.31	0	30,36,39	0.41	0
1	OMC	B5	1790	1,81	19,22,23	0.29	0	26,31,34	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PSU	A2	647	46	18,21,22	0.47	0	22,30,33	0.57	0
1	PSU	B5	4019	1	18,21,22	0.48	0	22,30,33	0.58	0
1	PSU	B5	3995	1	18,21,22	0.48	0	22,30,33	0.60	0
46	A2M	A2	27	46,81	22,25,26	0.06	0	31,36,39	0.27	0
1	A2M	B5	3307	1	22,25,26	0.08	0	31,36,39	0.37	0
1	PSU	B5	4343	1	18,21,22	0.48	0	22,30,33	0.59	0
46	A2M	A2	158	46	22,25,26	0.08	0	31,36,39	0.17	0
1	OMC	B5	2171	1,81	19,22,23	0.29	0	26,31,34	0.40	0
46	OMG	A2	470	46,81	23,26,27	0.28	0	33,38,41	0.39	0
46	OMG	A2	562	46	23,26,27	0.28	0	33,38,41	0.34	0
46	PSU	A2	610	46	18,21,22	0.46	0	22,30,33	0.61	0
46	PSU	A2	109	46,81	18,21,22	0.50	0	22,30,33	0.57	0
1	OMC	B5	2610	1	19,22,23	0.28	0	26,31,34	0.34	0
1	OMC	B5	3364	1	19,22,23	0.31	0	26,31,34	0.47	0
1	OMG	B5	2113	1	23,26,27	0.28	0	33,38,41	0.38	0
1	OMG	B5	3937	1	23,26,27	0.29	0	33,38,41	0.43	0
1	OMG	B5	3835	1	23,26,27	0.27	0	33,38,41	0.38	0
46	A2M	A2	165	46	22,25,26	0.08	0	31,36,39	0.39	0
46	OMU	A2	121	46	19,22,23	0.29	0	26,31,34	0.46	0
1	OMG	B5	3104	1	23,26,27	0.30	0	33,38,41	0.52	0
1	PSU	B5	4116	1	18,21,22	0.48	0	22,30,33	0.59	0
1	PSU	B5	3885	1	18,21,22	0.52	0	22,30,33	0.62	1 (4%)
1	A2M	B5	1780	1,81	22,25,26	0.08	0	31,36,39	0.48	0
1	PSU	B5	3964	1,81	18,21,22	0.51	0	22,30,33	0.59	0
46	OMC	A2	173	46	19,22,23	0.29	0	26,31,34	0.45	0
46	4AC	A2	1796	46	21,24,25	0.30	0	29,34,37	0.30	0
1	OMG	B5	4061	1	23,26,27	0.28	0	33,38,41	0.43	0
1	A2M	B5	2112	1,81	22,25,26	0.07	0	31,36,39	0.20	0
1	OMU	B5	3402	1	19,22,23	0.29	0	26,31,34	0.48	0
1	OMG	B5	3269	1	23,26,27	0.28	0	33,38,41	0.34	0
1	OMC	B5	3285	1	19,22,23	0.30	0	26,31,34	0.36	0
46	OMG	A2	644	46	23,26,27	0.33	0	33,38,41	0.38	0
1	PSU	B5	4022	1	18,21,22	0.49	0	22,30,33	0.57	0
46	A2M	A2	551	46	22,25,26	0.12	0	31,36,39	0.33	0
1	OMG	B5	1548	1,81	23,26,27	0.30	0	33,38,41	0.42	0
1	OMG	B5	3942	1	23,26,27	0.28	0	33,38,41	0.40	0
1	A2M	B5	1447	1	22,25,26	0.12	0	31,36,39	0.33	0
1	OMG	B5	3671	1	23,26,27	0.26	0	33,38,41	0.45	0
1	PSU	B5	4132	1	18,21,22	0.47	0	22,30,33	0.61	0
1	PSU	B5	3755	1	18,21,22	0.48	0	22,30,33	0.58	0
1	PSU	B5	3796	1	18,21,22	0.47	0	22,30,33	0.58	0
1	OMG	B5	2625	1	23,26,27	0.28	0	33,38,41	0.38	0
1	OMU	B5	3749	1	19,22,23	0.30	0	26,31,34	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	UY1	B5	3295	1,81	19,22,23	0.50	0	22,31,34	0.54	0
1	PSU	B5	1606	1,81	18,21,22	0.49	0	22,30,33	0.59	0
46	PSU	A2	782	46	18,21,22	0.60	1 (5%)	22,30,33	0.67	1 (4%)
1	OMG	B5	1445	1	23,26,27	0.29	0	33,38,41	0.48	0
1	A2M	B5	401	1	22,25,26	0.09	0	31,36,39	0.19	0
1	PSU	B5	1700	1	18,21,22	0.52	0	22,30,33	0.56	0
46	OMU	A2	389	46	19,22,23	0.32	0	26,31,34	0.50	0
46	PSU	A2	258	46	18,21,22	0.48	0	22,30,33	0.57	0
1	A2M	B5	2536	1,81	22,25,26	0.08	0	31,36,39	0.21	0
1	OMG	B5	3639	1	23,26,27	0.28	0	33,38,41	0.36	0
1	A2M	B5	1457	1,81	22,25,26	0.07	0	31,36,39	0.35	0
1	OMC	B5	2100	1	19,22,23	0.32	0	26,31,34	0.42	0
1	OMC	B5	2553	1	19,22,23	0.28	0	26,31,34	0.39	0
46	PSU	A2	642	46	18,21,22	0.49	0	22,30,33	0.59	0
1	PSU	B5	3742	1	18,21,22	0.50	0	22,30,33	0.56	0
46	MA6	A2	1805	46	23,26,27	0.31	0	34,38,41	0.67	1 (2%)
1	OMU	B5	4063	1	19,22,23	0.31	0	26,31,34	0.54	0
1	OMC	B5	1265	1	19,22,23	0.28	0	26,31,34	0.42	0
46	OMC	A2	1658	46	19,22,23	0.27	0	26,31,34	0.42	0
1	OMU	B5	2586	1	19,22,23	0.32	0	26,31,34	0.55	0
1	PSU	B5	1652	1	18,21,22	0.48	0	22,30,33	0.57	0
1	A2M	B5	4014	1	22,25,26	0.09	0	31,36,39	0.25	0
1	PSU	B5	3116	1	18,21,22	0.50	0	22,30,33	0.58	0
1	A2M	B5	3966	1,81	22,25,26	0.08	0	31,36,39	0.52	1 (3%)
46	OMG	A2	1286	46	23,26,27	0.28	0	33,38,41	0.37	0
1	OMG	B5	1241	1	23,26,27	0.33	0	33,38,41	0.49	0
46	PSU	A2	1039	46	18,21,22	0.60	1 (5%)	22,30,33	0.65	0
1	PSU	B5	4372	1,81	18,21,22	0.50	0	22,30,33	0.58	0
1	A2M	B5	399	1	22,25,26	0.08	0	31,36,39	0.23	0
43	MLZ	B ₀	53	43	8,9,10	0.73	0	4,9,11	0.64	0
1	PSU	B5	3172	1,81	18,21,22	0.49	0	22,30,33	0.60	0
46	OMU	A2	171	46	19,22,23	0.25	0	26,31,34	0.55	0
1	OMC	B5	3899	1	19,22,23	0.29	0	26,31,34	0.37	0
1	OMC	B5	3318	1	19,22,23	0.28	0	26,31,34	0.41	0
1	OMG	B5	2173	1	23,26,27	0.27	0	33,38,41	0.35	0
46	OMG	A2	1445	46,81	23,26,27	0.27	0	33,38,41	0.38	0
46	OMU	A2	116	46	19,22,23	0.28	0	26,31,34	0.42	0
46	PSU	A2	775	46	18,21,22	0.46	0	22,30,33	0.58	0
1	A2M	B5	3302	1	22,25,26	0.07	0	31,36,39	0.26	0
46	A2M	A2	99	46,81	22,25,26	0.08	0	31,36,39	0.29	0
1	OMC	B5	3346	1	19,22,23	0.28	0	26,31,34	0.44	0
1	OMU	B5	3670	1	19,22,23	0.31	0	26,31,34	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	6MZ	B5	3663	1	22,25,26	0.30	0	30,36,39	0.34	0
1	PSU	B5	3866	1	18,21,22	0.49	0	22,30,33	0.57	0
1	A2M	B5	3344	1	22,25,26	0.09	0	31,36,39	0.23	0
1	A2M	B5	4033	1	22,25,26	0.09	0	31,36,39	0.27	0
46	A2M	A2	629	46,81	22,25,26	0.11	0	31,36,39	0.28	0
1	PSU	B5	3900	1	18,21,22	0.51	0	22,30,33	0.59	1 (4%)
1	PSU	B5	3804	1	18,21,22	0.46	0	22,30,33	0.58	0
1	OMU	B5	3941	1	19,22,23	0.30	0	26,31,34	0.47	0
46	4AC	A2	1295	46	21,24,25	0.33	0	29,34,37	0.41	0
46	A2M	A2	445	46	22,25,26	0.07	0	31,36,39	0.25	0
1	A2M	B5	3262	1,81	22,25,26	0.11	0	31,36,39	0.47	0
46	PSU	A2	93	46	18,21,22	0.50	0	22,30,33	0.56	0
1	OMG	B5	3221	1	23,26,27	0.28	0	33,38,41	0.41	0
2	PSU	B8	55	2	18,21,22	0.45	0	22,30,33	0.61	0
1	OMG	B5	4066	1	23,26,27	0.30	0	33,38,41	0.49	0
46	OMU	A2	1284	46	19,22,23	0.24	0	26,31,34	0.47	0
1	UR3	B5	3973	1	19,22,23	0.30	0	26,32,35	0.31	0
46	PSU	A2	1132	46,81	18,21,22	0.48	0	22,30,33	0.58	0
76	NMM	As	67	76	9,11,12	1.59	1 (11%)	6,12,14	3.56	2 (33%)
1	PSU	B5	3114	1,81	18,21,22	0.45	0	22,30,33	0.63	0
2	PSU	B8	69	2,81	18,21,22	0.54	0	22,30,33	0.66	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	B5	3736	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	1771	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3195	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	1600	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3813	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	4071	1	-	0/7/25/26	0/2/2/2
60	IAS	An	138	60	-	3/7/7/8	-
1	PSU	B5	3397	1,81	-	0/7/25/26	0/2/2/2
1	PSU	B5	1769	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	3376	1,81	-	0/9/27/28	0/3/3/3
1	A2M	B5	1251	1	-	1/9/27/28	0/3/3/3
1	PSU	B5	3874	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3192	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	4080	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	B5	2564	1	-	0/9/27/28	0/3/3/3
46	OMG	A2	605	46	-	3/9/27/28	0/3/3/3
1	OMC	B5	3979	1	-	0/9/27/28	0/2/2/2
2	OMG	B8	75	2	-	0/9/27/28	0/3/3/3
46	OMU	A2	315	46	-	2/9/27/28	0/2/2/2
1	5MC	B5	3259	1,81	-	0/7/25/26	0/2/2/2
1	PSU	B5	3739	1	-	0/7/25/26	0/2/2/2
6	HIC	BB	245	6	-	0/5/6/8	0/1/1/1
1	1MA	B5	1247	1,81	-	2/7/25/26	0/3/3/3
1	PSU	B5	3975	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3846	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3201	1	-	1/9/27/28	0/3/3/3
46	MA6	A2	1804	46	-	0/11/29/30	0/3/3/3
46	A2M	A2	989	46	-	0/9/27/28	0/3/3/3
1	5MC	B5	3890	1	-	3/7/25/26	0/2/2/2
46	PSU	A2	774	46	-	3/7/25/26	0/2/2/2
1	OMC	B5	3178	1,81	-	4/9/27/28	0/2/2/2
46	A2M	A2	1341	46	-	1/9/27/28	0/3/3/3
46	B8N	A2	1206	46	-	4/16/34/35	0/2/2/2
1	PSU	B5	1690	1	-	0/7/25/26	0/2/2/2
46	6MZ	A2	1786	46,81	-	0/9/27/28	0/3/3/3
1	OMC	B5	1790	1,81	-	0/9/27/28	0/2/2/2
46	PSU	A2	647	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	4019	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3995	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	27	46,81	-	0/9/27/28	0/3/3/3
1	A2M	B5	3307	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4343	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	158	46	-	0/9/27/28	0/3/3/3
1	OMC	B5	2171	1,81	-	3/9/27/28	0/2/2/2
46	OMG	A2	470	46,81	-	0/9/27/28	0/3/3/3
46	OMG	A2	562	46	-	1/9/27/28	0/3/3/3
46	PSU	A2	610	46	-	0/7/25/26	0/2/2/2
46	PSU	A2	109	46,81	-	0/7/25/26	0/2/2/2
1	OMC	B5	2610	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3364	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2113	1	-	2/9/27/28	0/3/3/3
1	OMG	B5	3937	1	-	1/9/27/28	0/3/3/3
1	OMG	B5	3835	1	-	0/9/27/28	0/3/3/3
46	A2M	A2	165	46	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMU	A2	121	46	-	0/9/27/28	0/2/2/2
1	OMG	B5	3104	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4116	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3885	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	1780	1,81	-	0/9/27/28	0/3/3/3
1	PSU	B5	3964	1,81	-	2/7/25/26	0/2/2/2
46	OMC	A2	173	46	-	0/9/27/28	0/2/2/2
46	4AC	A2	1796	46	-	0/11/29/30	0/2/2/2
1	OMG	B5	4061	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	2112	1,81	-	1/9/27/28	0/3/3/3
1	OMU	B5	3402	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	3269	1	-	0/9/27/28	0/3/3/3
1	OMC	B5	3285	1	-	0/9/27/28	0/2/2/2
46	OMG	A2	644	46	-	0/9/27/28	0/3/3/3
1	PSU	B5	4022	1	-	0/7/25/26	0/2/2/2
46	A2M	A2	551	46	-	1/9/27/28	0/3/3/3
1	OMG	B5	1548	1,81	-	1/9/27/28	0/3/3/3
1	OMG	B5	3942	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	1447	1	-	1/9/27/28	0/3/3/3
1	OMG	B5	3671	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	4132	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3755	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3796	1	-	0/7/25/26	0/2/2/2
1	OMG	B5	2625	1	-	0/9/27/28	0/3/3/3
1	OMU	B5	3749	1	-	0/9/27/28	0/2/2/2
1	UY1	B5	3295	1,81	-	2/9/27/28	0/2/2/2
1	PSU	B5	1606	1,81	-	0/7/25/26	0/2/2/2
46	PSU	A2	782	46	-	0/7/25/26	0/2/2/2
1	OMG	B5	1445	1	-	0/9/27/28	0/3/3/3
1	A2M	B5	401	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	1700	1	-	0/7/25/26	0/2/2/2
46	OMU	A2	389	46	-	7/9/27/28	0/2/2/2
46	PSU	A2	258	46	-	0/7/25/26	0/2/2/2
1	A2M	B5	2536	1,81	-	3/9/27/28	0/3/3/3
1	OMG	B5	3639	1	-	1/9/27/28	0/3/3/3
1	A2M	B5	1457	1,81	-	2/9/27/28	0/3/3/3
1	OMC	B5	2100	1	-	3/9/27/28	0/2/2/2
1	OMC	B5	2553	1	-	0/9/27/28	0/2/2/2
46	PSU	A2	642	46	-	0/7/25/26	0/2/2/2
1	PSU	B5	3742	1	-	0/7/25/26	0/2/2/2
46	MA6	A2	1805	46	-	1/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	B5	4063	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	1265	1	-	0/9/27/28	0/2/2/2
46	OMC	A2	1658	46	-	0/9/27/28	0/2/2/2
1	OMU	B5	2586	1	-	0/9/27/28	0/2/2/2
1	PSU	B5	1652	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	4014	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3116	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3966	1,81	-	0/9/27/28	0/3/3/3
46	OMG	A2	1286	46	-	0/9/27/28	0/3/3/3
1	OMG	B5	1241	1	-	0/9/27/28	0/3/3/3
46	PSU	A2	1039	46	-	1/7/25/26	0/2/2/2
1	PSU	B5	4372	1,81	-	0/7/25/26	0/2/2/2
1	A2M	B5	399	1	-	1/9/27/28	0/3/3/3
43	MLZ	Bo	53	43	-	3/7/8/10	-
1	PSU	B5	3172	1,81	-	0/7/25/26	0/2/2/2
46	OMU	A2	171	46	-	0/9/27/28	0/2/2/2
1	OMC	B5	3899	1	-	0/9/27/28	0/2/2/2
1	OMC	B5	3318	1	-	0/9/27/28	0/2/2/2
1	OMG	B5	2173	1	-	0/9/27/28	0/3/3/3
46	OMG	A2	1445	46,81	-	1/9/27/28	0/3/3/3
46	OMU	A2	116	46	-	2/9/27/28	0/2/2/2
46	PSU	A2	775	46	-	0/7/25/26	0/2/2/2
1	A2M	B5	3302	1	-	0/9/27/28	0/3/3/3
46	A2M	A2	99	46,81	-	0/9/27/28	0/3/3/3
1	OMC	B5	3346	1	-	1/9/27/28	0/2/2/2
1	OMU	B5	3670	1	-	0/9/27/28	0/2/2/2
1	6MZ	B5	3663	1	-	0/9/27/28	0/3/3/3
1	PSU	B5	3866	1	-	0/7/25/26	0/2/2/2
1	A2M	B5	3344	1	-	1/9/27/28	0/3/3/3
1	A2M	B5	4033	1	-	1/9/27/28	0/3/3/3
46	A2M	A2	629	46,81	-	3/9/27/28	0/3/3/3
1	PSU	B5	3900	1	-	0/7/25/26	0/2/2/2
1	PSU	B5	3804	1	-	0/7/25/26	0/2/2/2
1	OMU	B5	3941	1	-	0/9/27/28	0/2/2/2
46	4AC	A2	1295	46	-	2/11/29/30	0/2/2/2
46	A2M	A2	445	46	-	0/9/27/28	0/3/3/3
1	A2M	B5	3262	1,81	-	2/9/27/28	0/3/3/3
46	PSU	A2	93	46	-	0/7/25/26	0/2/2/2
1	OMG	B5	3221	1	-	0/9/27/28	0/3/3/3
2	PSU	B8	55	2	-	0/7/25/26	0/2/2/2
1	OMG	B5	4066	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	OMU	A2	1284	46	-	0/9/27/28	0/2/2/2
1	UR3	B5	3973	1	-	0/7/25/26	0/2/2/2
46	PSU	A2	1132	46,81	-	0/7/25/26	0/2/2/2
76	NMM	As	67	76	-	5/9/11/13	-
1	PSU	B5	3114	1,81	-	0/7/25/26	0/2/2/2
2	PSU	B8	69	2,81	-	0/7/25/26	0/2/2/2

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
76	As	67	NMM	CZ-NH2	4.34	1.44	1.34
6	BB	245	HIC	CD2-CG	3.04	1.41	1.36
1	B5	1600	PSU	O4'-C1'	-2.35	1.40	1.43
46	A2	782	PSU	O4'-C1'	-2.17	1.40	1.43
46	A2	1039	PSU	O4'-C1'	-2.16	1.40	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	As	67	NMM	NE-CZ-NH2	-7.62	112.49	119.48
76	As	67	NMM	NE-CZ-NH1	4.12	127.97	120.26
46	A2	1804	MA6	C2-N1-C6	2.46	117.57	111.75
46	A2	1805	MA6	C2-N1-C6	2.42	117.46	111.75
60	An	138	IAS	OD1-CG-CB	-2.40	118.43	125.43

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B5	2171	OMC	C1'-C2'-O2'-CM2
1	B5	3178	OMC	C2'-C1'-N1-C2
1	B5	3178	OMC	C2'-C1'-N1-C6
1	B5	3201	A2M	C1'-C2'-O2'-CM'
1	B5	3639	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

48 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	3195	A2M	5	0
1	B5	4071	PSU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	1251	A2M	1	0
1	B5	3874	PSU	2	0
1	B5	3979	OMC	1	0
2	B8	75	OMG	2	0
46	A2	315	OMU	4	0
1	B5	3201	A2M	2	0
1	B5	3890	5MC	2	0
46	A2	774	PSU	1	0
46	A2	1341	A2M	1	0
46	A2	27	A2M	1	0
46	A2	158	A2M	1	0
1	B5	2171	OMC	1	0
46	A2	470	OMG	1	0
46	A2	562	OMG	1	0
46	A2	610	PSU	1	0
46	A2	109	PSU	1	0
1	B5	2610	OMC	1	0
1	B5	3364	OMC	1	0
1	B5	2113	OMG	1	0
1	B5	3937	OMG	1	0
1	B5	3835	OMG	2	0
46	A2	121	OMU	1	0
1	B5	1780	A2M	1	0
1	B5	4061	OMG	1	0
1	B5	2112	A2M	1	0
1	B5	4022	PSU	2	0
1	B5	3671	OMG	1	0
1	B5	2625	OMG	2	0
1	B5	3749	OMU	1	0
1	B5	3295	UY1	1	0
1	B5	1606	PSU	1	0
1	B5	2100	OMC	1	0
1	B5	4063	OMU	2	0
1	B5	1265	OMC	1	0
46	A2	1658	OMC	2	0
1	B5	4372	PSU	1	0
46	A2	1445	OMG	1	0
46	A2	116	OMU	1	0
46	A2	99	A2M	1	0
1	B5	3663	6MZ	1	0
1	B5	3344	A2M	1	0
1	B5	3900	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B5	3941	OMU	1	0
46	A2	1295	4AC	2	0
1	B5	3262	A2M	2	0
1	B5	3973	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 501 ligands modelled in this entry, 501 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

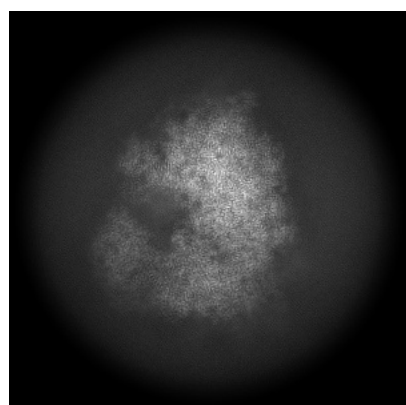
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18168. These allow visual inspection of the internal detail of the map and identification of artifacts.

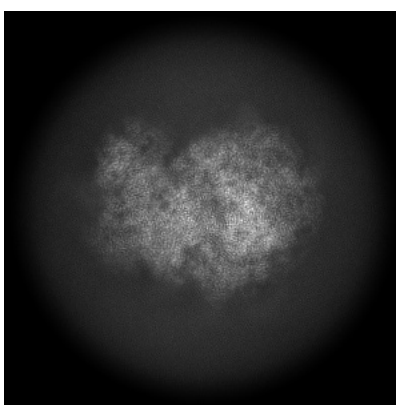
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

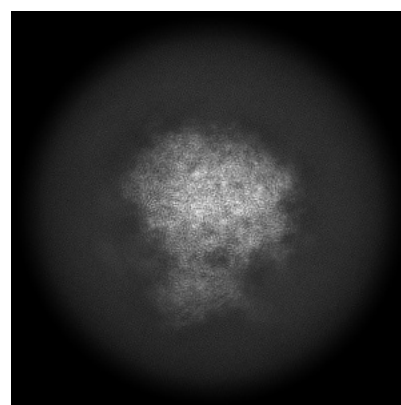
6.1.1 Primary map



X



Y



Z

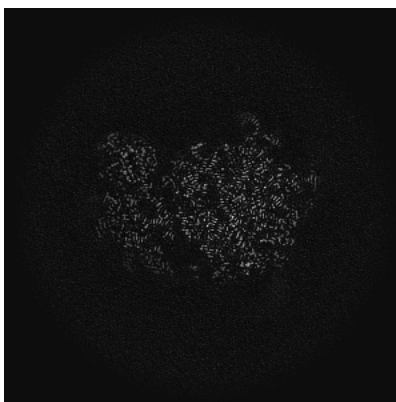
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

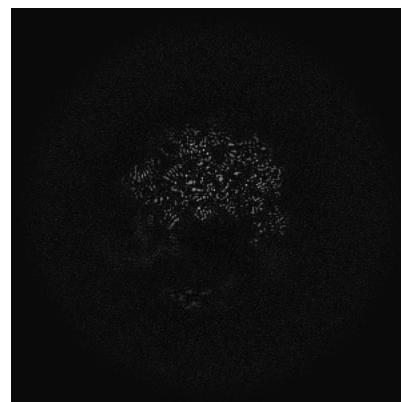
6.2.1 Primary map



X Index: 290



Y Index: 290

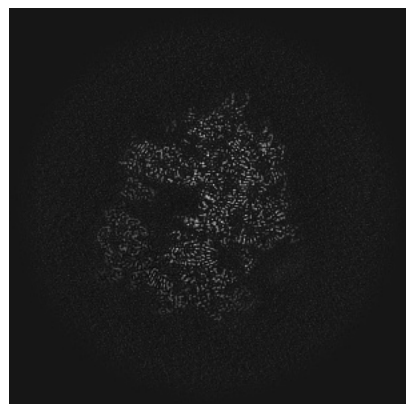


Z Index: 290

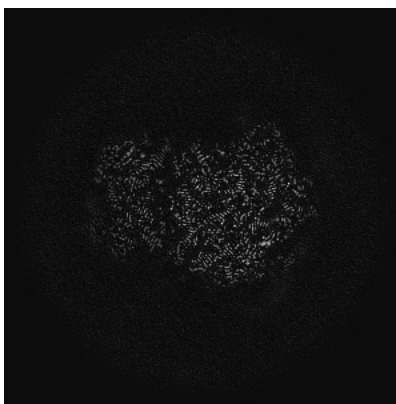
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

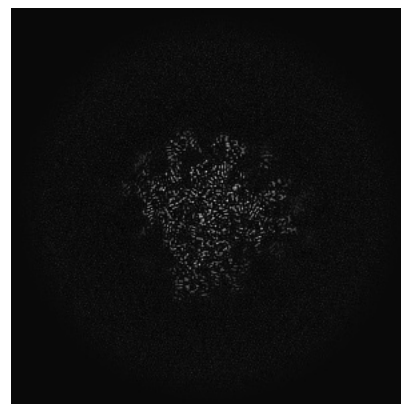
6.3.1 Primary map



X Index: 270



Y Index: 300

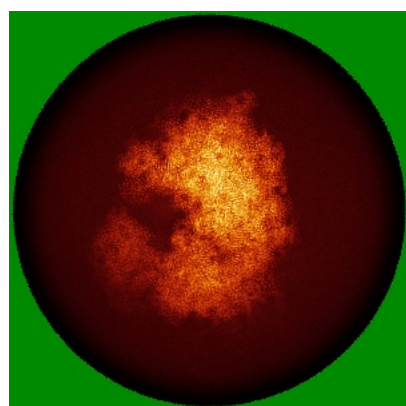


Z Index: 348

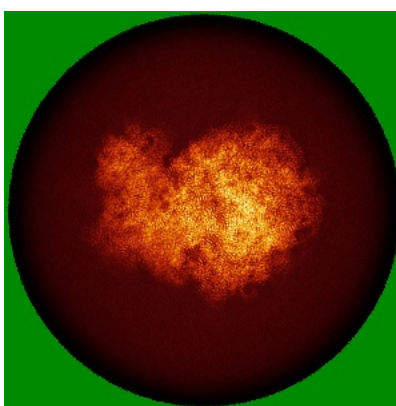
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

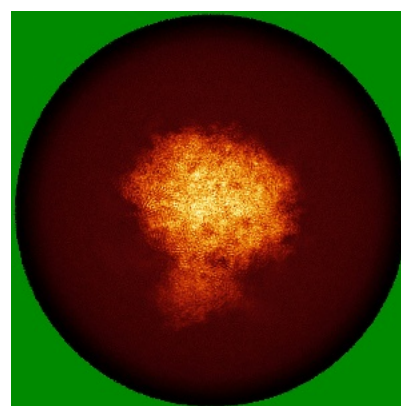
6.4.1 Primary map



X



Y

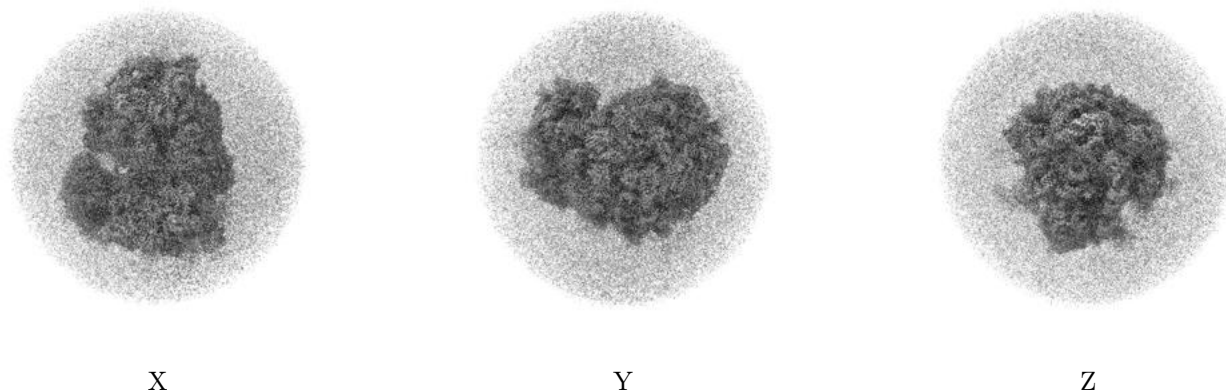


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

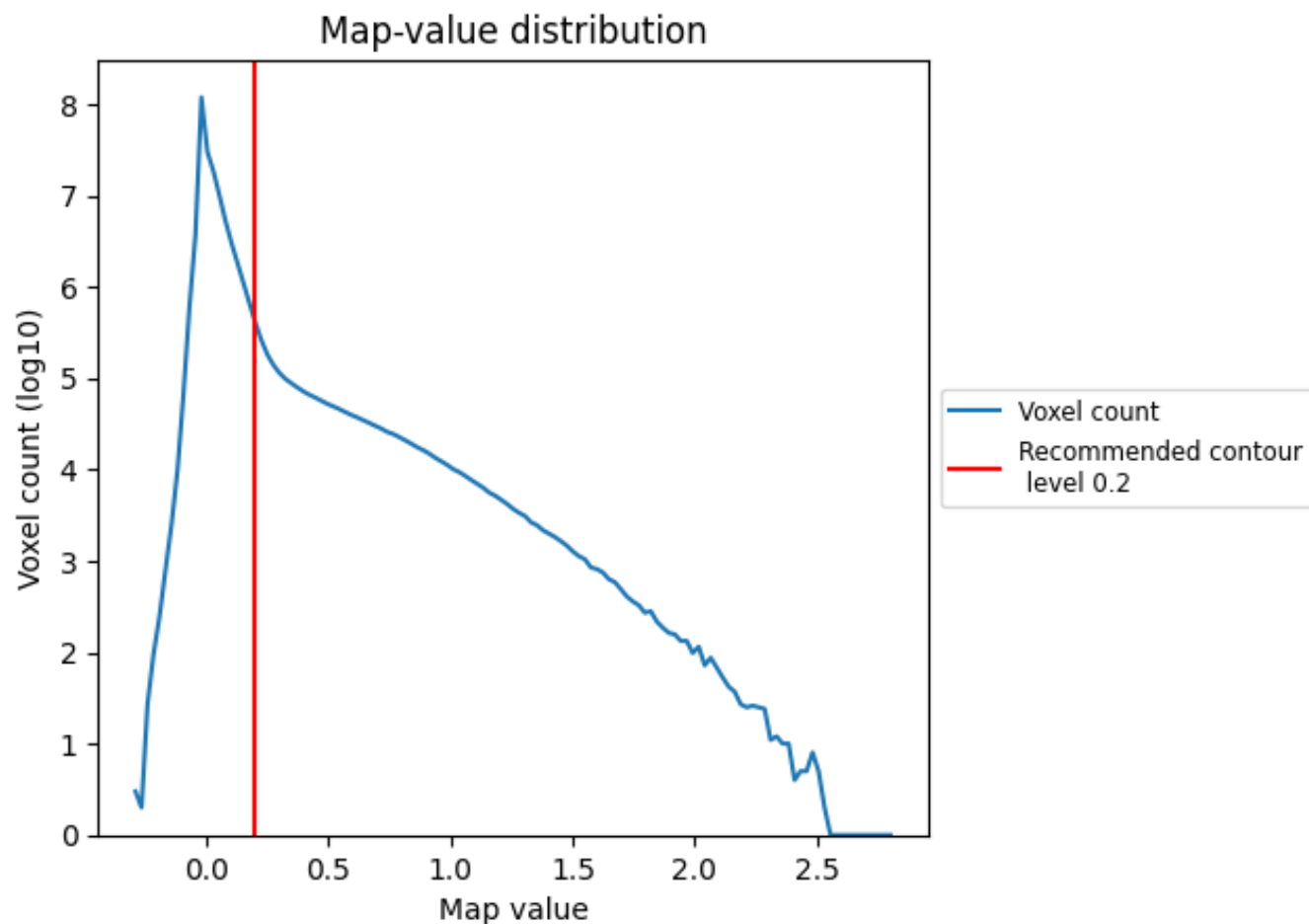
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

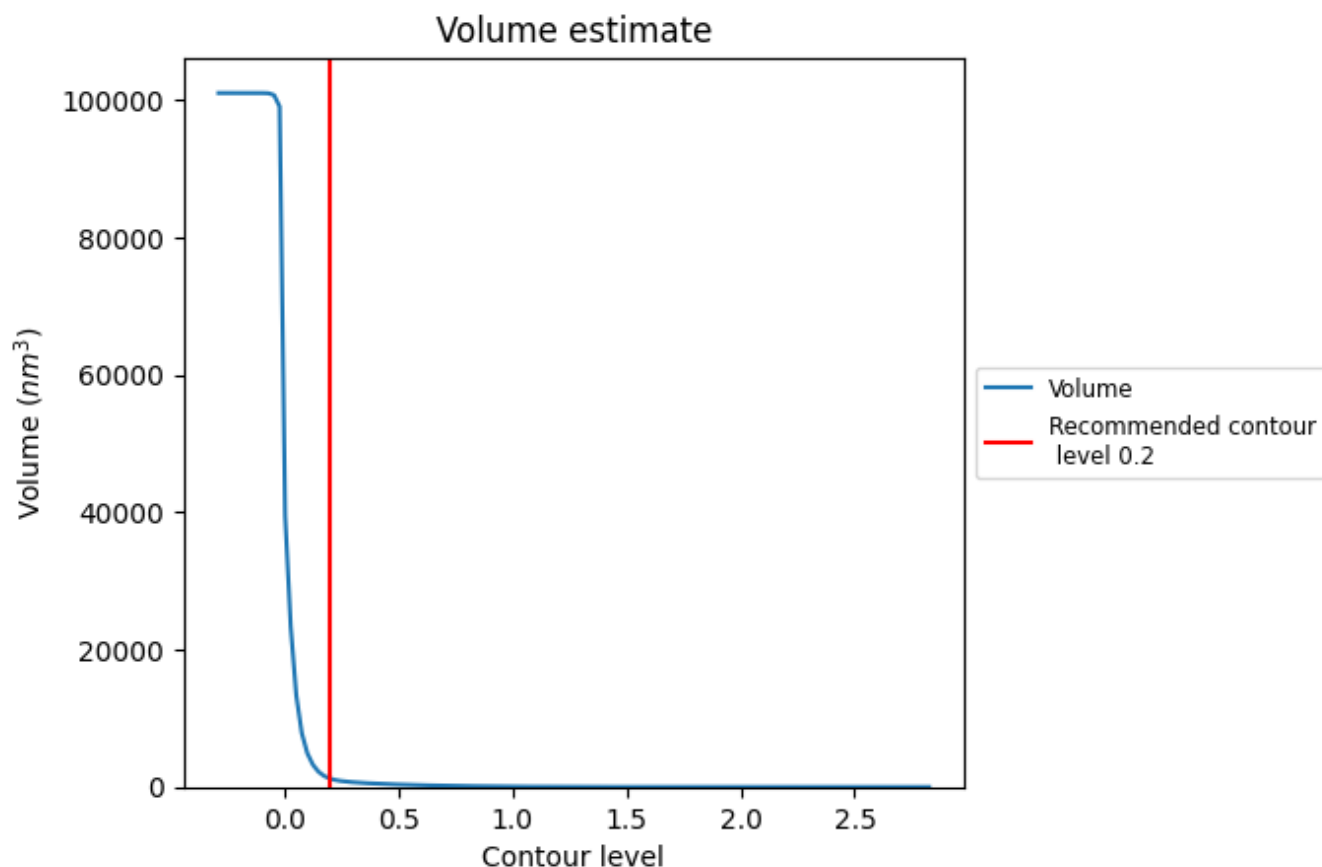
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

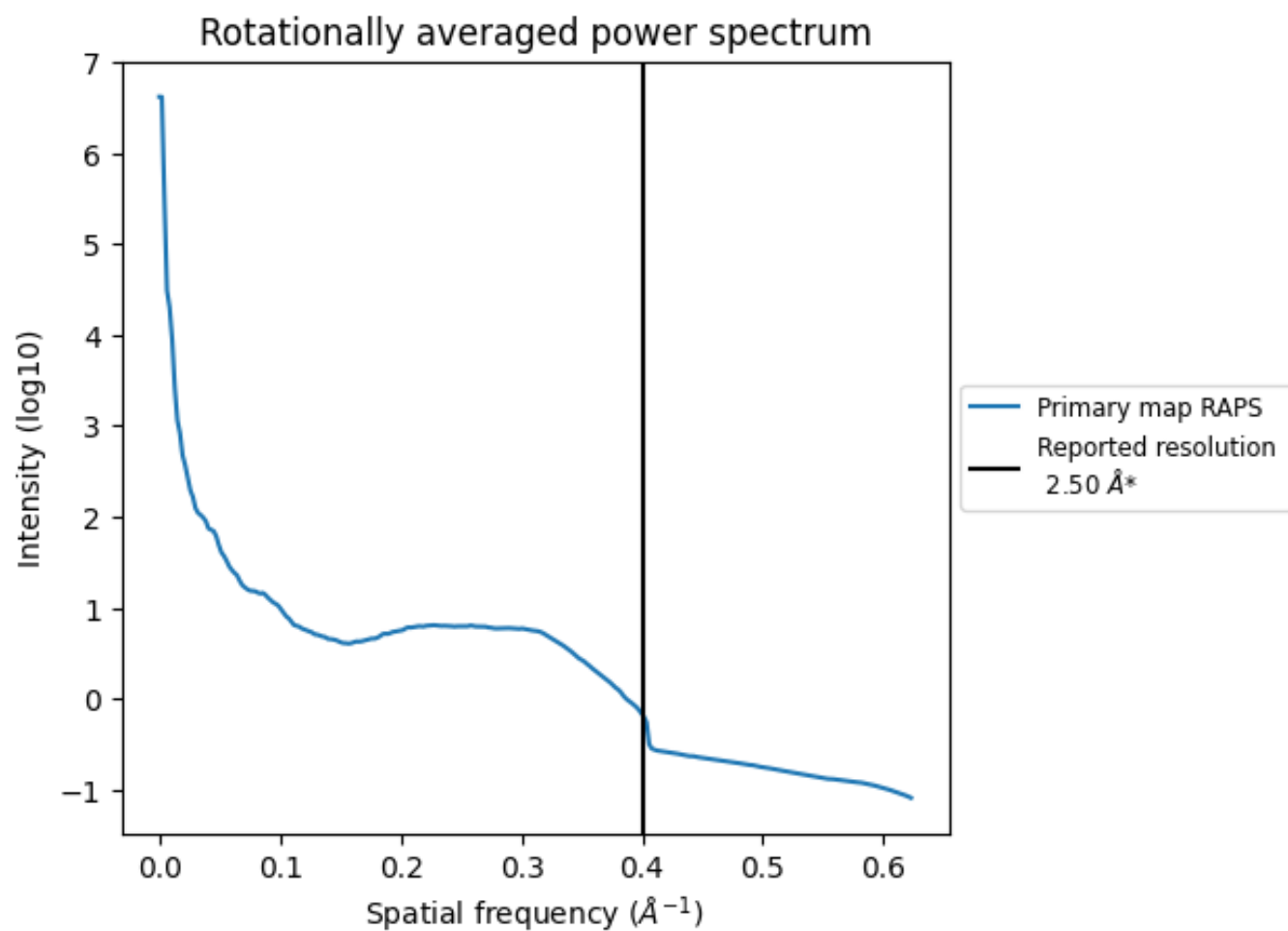
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1226 nm³; this corresponds to an approximate mass of 1108 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

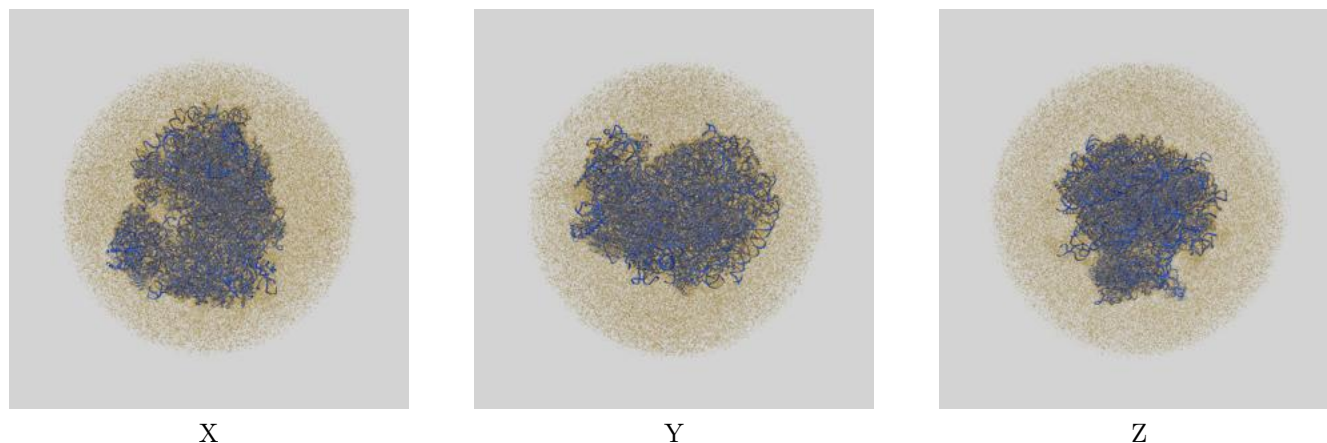
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

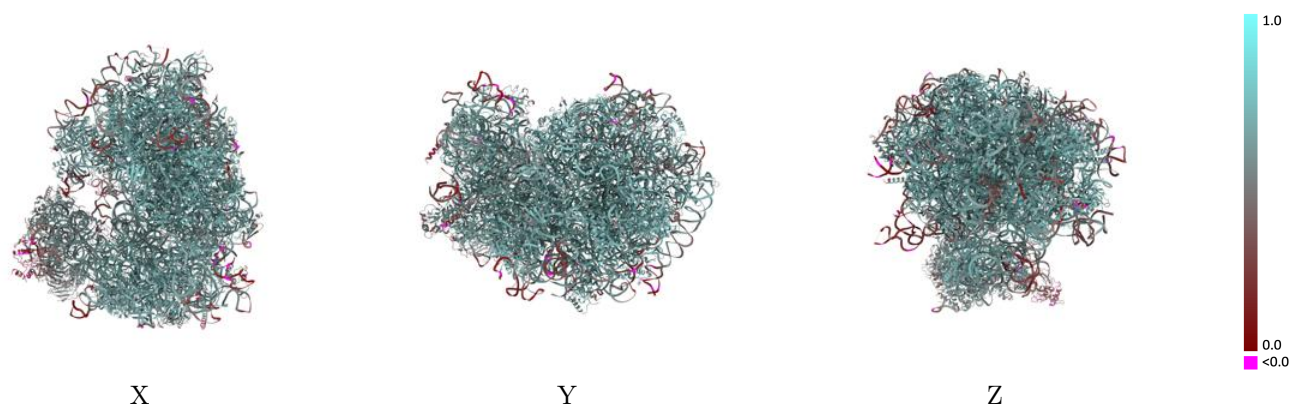
This section contains information regarding the fit between EMDB map EMD-18168 and PDB model 8Q7Z. Per-residue inclusion information can be found in section [3](#) on page [25](#).

9.1 Map-model overlay [i](#)



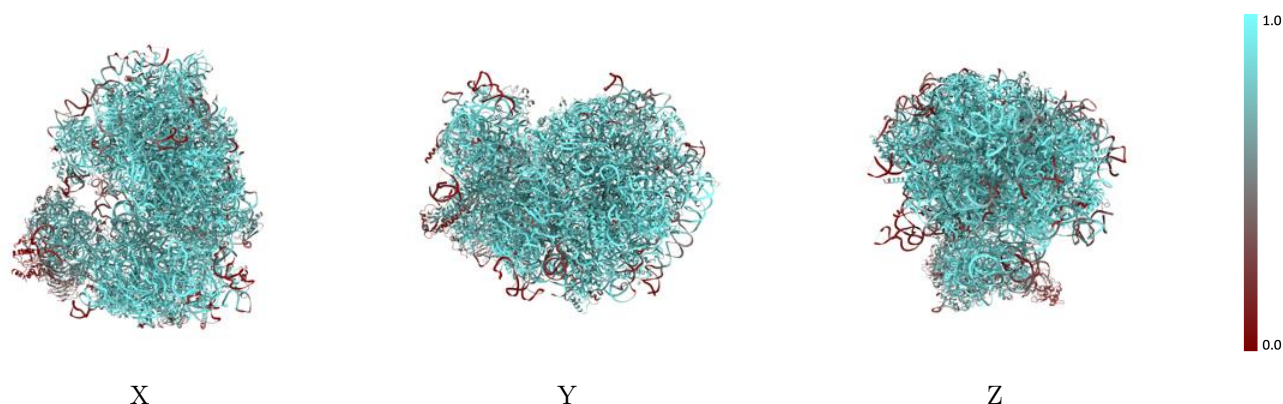
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



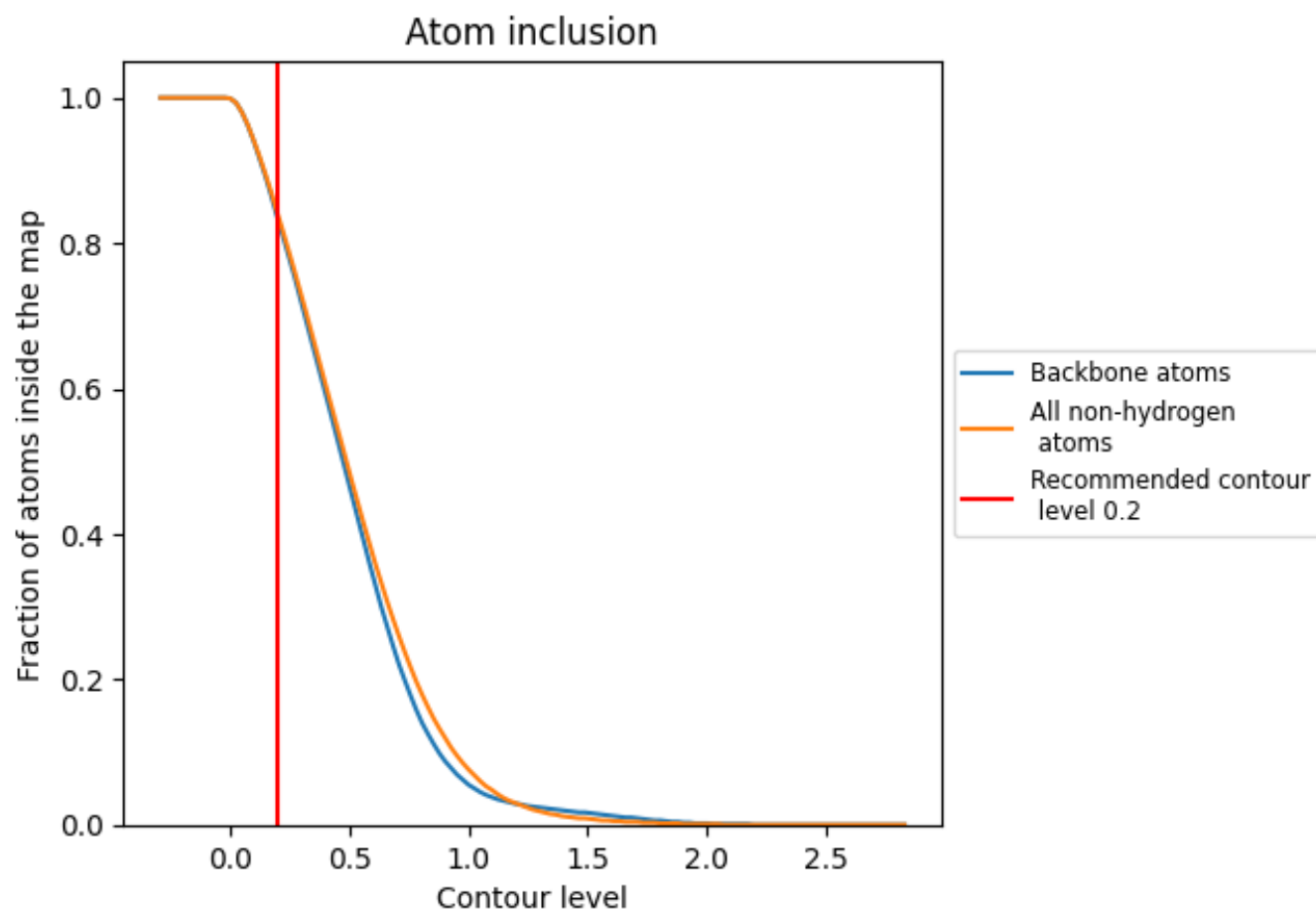
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8420	 0.6160
A2	 0.8570	 0.5980
AA	 0.7270	 0.5760
AB	 0.5470	 0.5230
AC	 0.0390	 0.2340
AD	 0.6930	 0.5710
AE	 0.8700	 0.6600
AF	 0.3390	 0.4560
AG	 0.7830	 0.5950
AZ	 0.7970	 0.6150
Aa	 0.8260	 0.6260
Ab	 0.8670	 0.6510
Ac	 0.5510	 0.5170
Ad	 0.9170	 0.6570
Ae	 0.6880	 0.5580
Af	 0.7370	 0.5630
Ag	 0.4980	 0.5000
Ah	 0.8280	 0.6260
Ai	 0.9040	 0.6480
Aj	 0.5370	 0.4940
Ak	 0.8490	 0.6430
Al	 0.0370	 0.1750
Am	 0.8760	 0.6570
An	 0.8480	 0.6360
Ao	 0.6100	 0.5240
Ap	 0.7430	 0.5710
Aq	 0.5090	 0.4910
Ar	 0.6520	 0.5250
As	 0.7210	 0.5640
At	 0.5200	 0.4930
Au	 0.8220	 0.6340
Av	 0.9390	 0.6780
Aw	 0.8880	 0.6570
Ax	 0.8710	 0.6350
Ay	 0.5310	 0.4860



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Chain	Atom inclusion	Q-score
Az	 0.9080	 0.6760
B5	 0.8680	 0.6130
B7	 0.9750	 0.6660
B8	 0.9150	 0.6420
BA	 0.9740	 0.7140
BB	 0.9450	 0.6970
BC	 0.9460	 0.6910
BD	 0.8490	 0.6340
BE	 0.8670	 0.6410
BF	 0.9480	 0.7040
BG	 0.8200	 0.6240
BH	 0.9100	 0.6640
BI	 0.9190	 0.6740
BJ	 0.7960	 0.6130
BL	 0.8780	 0.6500
BM	 0.9390	 0.6820
BN	 0.9880	 0.7210
BO	 0.9470	 0.6880
BP	 0.9440	 0.6960
BQ	 0.9700	 0.7140
BR	 0.8300	 0.6260
BS	 0.9650	 0.7020
BT	 0.9000	 0.6770
BU	 0.6920	 0.5570
BV	 0.9460	 0.7040
BW	 0.8520	 0.6440
BX	 0.9070	 0.6730
BY	 0.9190	 0.6660
BZ	 0.8970	 0.6590
Ba	 0.9750	 0.7190
Bb	 0.8190	 0.6220
Bc	 0.9170	 0.6690
Bd	 0.8960	 0.6670
Be	 0.9630	 0.7080
Bf	 0.9610	 0.7170
Bg	 0.9240	 0.6820
Bh	 0.9020	 0.6650
Bi	 0.8940	 0.6560
Bj	 0.9780	 0.7030
Bk	 0.7090	 0.5970
Bl	 0.9080	 0.6780
Bm	 0.9300	 0.6810

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Chain	Atom inclusion	Q-score
Bo	 0.9070	 0.6850
Bp	 0.9270	 0.6870
Br	 0.9320	 0.6860
V	 0.3470	 0.3090